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Technical Activities 1984

Office of Standard Reference Data

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Technical Activities 1984

Office of Standard Reference Data

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U.S. DEPARTMENT OF COMMERCE
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ABSTRACT

The Office of Standard Reference Data is one of two program offices in the National Measurement Laboratory, National Bureau of Standards. The Standard Reference Data Program develops and disseminates databases of critically evaluated physical, chemical, and materials properties of substances. These databases are available through NBS and private publications, on magnetic tape, and from online retrieval systems.

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the program for the year 1984.

Key words: chemical data; data compilation; evaluated data; materials properties data; numerical database; physical data; standard reference data; technical activities 1984

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INTRODUCTION

The Office of Standard Reference Data is responsible for program management and coordination of the National Standard Reference Data System (NSRDS). The major aim of the program is to provide critically evaluated numerical data to the scientific and technical community in a convenient and accessible form. Certain secondary outputs, such as annotated bibliographies and procedures for computerized handling of data, are also made available. A second aim is to provide feedback into experimental programs to help raise the general standards of measurement. That is, by communicating the experience gained in evaluating the world output of data in the physical sciences, NSRDS helps to advance the level of experimental techniques and improve the reliability of physical measurements.

The formal existence of the NSRDS dates from 1963, when the Federal Council for Science and Technology asked the National Bureau of Standards to assume primary responsibility in the Federal Government for promoting and coordinating the critical evaluation of numerical data in the physical sciences. The program was conceived as a decentralized national effort, with financial support coming from a variety of Government and private sources, but with NBS responsible for the overall planning and coordination. In 1968 the Congress provided a specific legislative mandate for the program through passage of Public Law 90-396, the Standard Reference Data Act.* This Act states the policy of the Congress to make reliable reference data available to scientists, engineers, and the general public, and it encourages cooperation among NBS, other Federal Agencies, and the private sector in meeting this objective.

The technical scope of the program gives primary emphasis to well-defined physical and chemical properties of substances and systems which are well characterized. Also included are materials of commerce (alloys, ceramics, etc.) whose composition may vary only within clearly stated ranges. Materials of uncertain or widely variable composition are not included. Properties which depend upon arbitrarily defined characteristics of the measurement technique are generally excluded. While these definitions leave many border-line cases, the overall intent is to concentrate the effort on intrinsic properties that are clearly defined in terms of accepted physical theory and substances whose composition and history are so well known as to justify evaluation of the data. Biological properties and data relating to large natural systems (e.g., the atmosphere, the oceans) also fall outside the program.

The Office of Standard Reference Data monitors and coordinates the work of the various data centers and specialized projects which collectively make up the NSRDS. These projects are located in the technical divisions of NBS and in universities, industrial laboratories, and other Government laboratories. Close association between data evaluation projects and relevant experimental research programs helps provide the critical judgment which is essential to assure the reliability of the final output.

*See Appendix G

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The principal output of the program consists of compilations of evaluated data and critical reviews of the status of data in particular technical areas. Evaluation of data implies a careful examination, by an experienced specialist, of all published measurements of the quantity in question, leading to the selection of a recommended value and statement concerning its accuracy or reliability. The techniques of evaluation depend upon the data in question, but generally include an examination of the method of measurement and the characterization of the materials, a comparison with relevant data on other properties and materials, and a check for consistency with theoretical relationships. Adequate documentation is provided for the selection of recommended values and accuracy estimates.

Evaluated data produced under the NSRDS program are disseminated through the following mechanisms:

Journal of Physical and Chemical Reference Data - A quarterly journal containing data compilations and critical data reviews, published for the National Bureau of Standards by the American Institute of Physics and the American Chemical Society.

NSRDS-NBS Series - A publication series distributed by the Superintendent of Documents, U.S. Government Printing Office.

Appropriate publications of technical societies and commercial publishers.

Magnetic tapes, on-line networks, and other computer-based formats.

Response by OSRD and individual data centers to inquiries for specific data.

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PROGRAM STRUCTURE

Current activities in the Standard Reference Data program are carried out in 25 data centers and approximately 30 short-term projects located in the technical divisions of NBS and in academic and industrial laboratories. Each of these activities undertakes the collection and evaluation of the available data on a specified set of properties and substances. The activities are aggregated into three discipline-oriented program areas:

Physical Data - Includes data on atomic, molecular, and nuclear properties, and spectral data utilized for chemical identification.

Chemical Data - Covers primarily kinetic, thermodynamic, and transport properties of substances important to the chemical and related industries.

Materials Properties Data - Includes structural, electrical, optical, and mechanical properties of solid materials of broad interest.

Since comprehensive coverage of all properties and materials of importance in these three program areas is not feasible, the Office of Standard Reference Data (OSRD) selects data sets of highest priority, based upon the present and anticipated applications of the data. The current focus in each area is described in the sections below.

In addition to its planning and coordinating role, OSRD is responsible for dissemination of the results from the projects that it supports. The principal means for dissemination is still hard-copy publications, although computer-based distribution is becoming more important, as described below. Response to specific inquiries for data directed to OSRD and the individual data centers forms another dissemination mode.

The following tables summarize the published output of the program and the distribution of this output:

Publications in 1984

Series	Pages Published	Titles Published
JPCRD, Vol. 13	1486	27
Data Compilations from other publishers	2320	2

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Publications in 1984 (cont.)

Series	Pages Published	Titles Published
Other Publications in NBS Series	250	2
Bibliographies and indexes from other publishers	900	2
Totals	4956	33

Subscribers to JPCRD

Month/Year	Number
9/1980	1234
9/1981	1265
9/1982	1234
9/1983	1230
9/1984	1186

Inquiries Received in OSRD

(Does not include inquiries received by data centers)

Year	Number
1980	787
1981	657
1982	613
1983	1022
1984*	616

Sales of JPCRD Offprints and Supplements

Year	Offprints	Supplements
1980	5079	111
1981	4254	137
1982	3567	266
1983	3081	1666
1984*	2900	1300

* Projected to end of year

PHYSICAL DATA

S. P. Fivozinsky, Program Manager

The Physical Data Program was created this year as the result of a change in the technical management structure within OSRD. The old programmatic areas, Energy and Environmental Data, and Industrial Process Data, have been reorganized to reflect a disciplinary content rather than application areas. As a result, the new Physical Data Program is concerned with atomic, molecular, nuclear, and those spectral databases used heavily in analytical chemical instrumentation.

The new Chemical Data Program emphasizes thermodynamics, thermophysical properties, kinetics, and other data which is chemical in nature. That Program will be described beginning on page 8.

Data centers and projects have been shifted to the control of different Program Managers to reflect these changes. The following data centers are associated with the Physical Data Program:

* Atomic Collisions Cross Section Data Center (CBS, JILA)
* Atomic Energy Levels Data Center (CRR)
* Atomic Transition Probabilities Data Center (CRR)
* Fundamental Constants Data Center (CBS)
* Molecular Spectra Data Center (CCP)
* Photon and Charged Particle Data Center (CRR)

These data centers are long-term activities which develop, maintain, and disseminate a major database in these areas. The Physical Data Program also supports a number of short-term projects whose efforts lead to specific one-time outputs. The following projects have been active during this calendar year:

* Critical Compilation of Mass Spectral Data
* Compilation of Atomic Wavelengths below 2000 A
* K shell Ionization by Hydrogen and Helium Ions
* Digitization of the Coblentz Society Infrared Database
* Soft X-ray Interactions with Matter
* Medical Physics Data Book, 2nd edition

Through the combination of data centers and short term projects the Physical Data Program addresses the most critical needs for databases with a combination of NBS and other-agency funding. More detailed descriptions of the data centers, the short-term projects, and their current activities and future plans, are found later in this report.

While most outputs of the Program are in printed form, an increasing number of computer-readable databases are being designed and disseminated.

In the future, internal operations of data centers, evaluation techniques, and dissemination will involve heavy utilization of modern computer technology.

Because of considerable increased pressure from user communities for greater support of these programs and availability of evaluated atomic and molecular data, a major effort will be made next year to develop new funding sources for this work and to draw increased attention to NBS as the primary national source for evaluated databases of atomic and molecular data.

Highlights of Recent Activities

The Physical Data Program has been very active during the last year. Two new projects have begun with a combination of NBS and other-agency funding. The first will expand the Photon and Charged Particle Data Center to carry out a pilot project to evaluate soft x-ray cross sections. A quantitative knowledge of low energy x-ray interactions with matter has many applications in understanding the effects of radiation on living tissue, in material science and in microcircuitry.

The second new project will expand the activities of the Atomic Energy Levels Data Center to include the compilation of wavelengths of atomic transitions. These are used heavily in identification of the specific atomic ions giving rise to a set of measured spectra. Initially the Data Center will compile magnetic dipole transitions since they are the ones primarily observed by astronomers, and measured during diagnostics of nuclear fusion plasmas.

The Atomic Energy Levels and Atomic Transition Probabilities Data Centers are presently working on the development of a computer-readable database. There has been considerable interest in the availability of such a system expressed by the scientific community through, for example, the NAS/NRC Committee on Line Spectra of the Elements, and members of the NAS Board on Assessment for the National Bureau of Standards.

The Fundamental Constants Data Center will publish the latest "Least Squares Adjustment of the Fundamental Constants." This effort represents the primary source of information in the world on the values of the fundamental physical constants. The new set of recommended values will be published as a CODATA Bulletin. The full details of the adjustment will be submitted for separate publication during FY 1985.

This year the Atomic Collisions Cross Section Data Center at JILA in Boulder, Colorado, will begin preparing a computerized database of electron collision cross sections for atoms, ions, and molecules. These data are important in modeling gas discharges and plasma systems such as those describing nuclear fusion processes and interstellar atmospheres.

The Molecular Spectra Data Center will be concentrating on a compilation of recommended rest frequencies of interstellar molecular transitions in the microwave region, and an infrared spectral calibration atlas. Microwave spectral data are the key to analyses of interstellar data coming from radio-telescopes. The infrared data are used by NASA for determination of chemical species in the stratosphere.

The Photon and Charged Particle Data Center has had a long and successful history of providing photon and electron interaction cross sections for varied applications in medicine, health physics, and national defense. This year the Center is releasing two computer-readable databases, EPSTAR, providing electron and positron stopping power data for 285 materials, and XGAM, an interactive system which calculates photon interaction cross sections on whatever substance the user inputs.

Other agency funded activities will lead this year to a major compilation of atomic wavelengths below 2000 A, a digitized database of reference condensed-phase infrared spectra, and a compilation of K shell ionization data. The Program continues to support the generation of new spectra for the Mass Spectral Database, which is widely disseminated. Plans are underway to develop a specific interagency agreement for future development of this database and other important spectral substance-identifying database systems.

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CHEMICAL DATA

H. J. White, Jr. Program Manager

With the retirement of Dr. Gevantman, the program on industrial process data was reorganized to become the program on chemical data. In the process, the activities on thermodynamics and transport properties which composed the program on industrial process data were augmented by centers and projects on chemical kinetics and molten salts.

These additions fit well with the previous program. The principal products of the Ion Kinetics and Energetics Data Center include the chemical thermodynamic properties of gaseous ions and highly reactive molecular fragments which complement and extend the data of the Chemical Thermodynamics Data Center. The kinetics data of this center, the Chemical Kinetics Information Center and the Radiation Chemistry Data Center complement the thermodynamics data. They can be used to obtain properties for transition-state species and are usually used with thermodynamic data for stable species in solving a variety of kinetic problems. The Molten Salt Data Center evaluates equilibrium and transport property data for molten salt systems. These complement and extend the data on aqueous salt systems evaluated by the Aqueous Electrolyte Data Center.

The program in chemical data is configured to provide evaluated data for a variety of thermodynamic, kinetic and transport properties. These include the enthalpy changes and equilibrium constants for a wide range of chemical reactions, the equations of state and thermodynamic properties of fluids, the kinetics of homogeneous reactions in fluid systems, and the viscosity, thermal conductivity and electrical conductivity of a large number of systems.

A number of major new products have appeared or are about to appear this year. One of them is Heat Capacities and Entropies of Organic Compounds in the Condensed Phase by E. S. Domalski, W. H. Evans and E. D. Hearing. This is Supplement No. 1 of Volume 13 of the Journal of Physical and Chemical Reference Data and contains data on approximately 1400 organic compounds. Another is the NBS/NRC Steam Tables by L. Haar, J. S. Gallagher and G. S. Kell which was published by Hemisphere Press. The formulation presented in this book provides an accurate representation of the data for the thermodynamic properties of water and steam from the triple point to 1000°C and for pressures up to, at least, 10k bars. It was accepted as the Provisional IAPS Formulation 1982 for the Thermodynamic Properties of Ordinary Water Substance for Scientific and General Use by the International Association for the Properties of Steam and forms the basis of the IAPS Formulation 1984 for the Thermodynamic Properties of Ordinary Water Substance for Scientific and General Use which is the current IAPS-accepted formulation.

In keeping with the emphasis on automation, two automated products have been prepared. One is a tape containing the NBS Chemical Thermodynamics Data Base. This tape contains software which will lead the user to properties for any of the 14000 items listed in a simple and quick way. The data base was published as a Supplement to the Journal of Physical and Chemical Reference Data in 1982.

The other is a searchable tape of the first 198 compounds in the DIPPR Data Compilation. This compilation, which will contain 1000 or more compounds when it is completed, is being produced at Penn State University with support from about 40 industrial organizations and NBS through the Design Institute for Physical Properties Data of the American Institute of Chemical Engineers (AIChE). The compilation will be published by AIChE; the interactive tape form was prepared with the support of NBS and will be marketed through OSRD. It is expected to become available before the end of 1984. Addition of this tape will bring the number of tape products available from this program to 5.

Another publication, which is in draft form, is the "CODATA Thermodynamic Tables. Tentative Selections for Some Compounds of Calcium and Related Mixtures (A Prototype Set of Tables)." These have been produced by the CODATA Task Group on Chemical Thermodynamic Tables and represent a departure from previous tables for several reasons. First, they have been produced by a decentralized international group but are internally consistent thermodynamically. Second, they can be added to and updated without destroying the internal consistency. Finally, they represent a draft of what the CODATA Task Group hopes will become an internationally accepted format for chemical thermodynamic tables. They are being sent out for review and comment. If the Prototype Tables meet with basic acceptance in the thermodynamic community, the Task Group intends to use them and as the basis for a comprehensive consistent set of internationally accepted chemical thermodynamic tables.

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MATERIALS PROPERTIES DATA

J. R. Rumble, Jr., Program Manager

The past year has been a challenging one for the Materials Properties Data Program. Highlights include major compilations of evaluated data, cooperative agreements on joint data activities with technical societies, and new data evaluation activities. The program has five components as shown in Table 1. In each area, projects are underway and new activities are planned, depending on funding.

Table 1

OSRD Materials Properties Data Program
Structure and Characterization
Physical Properties
Phase Equilibria
Performance Properties
Corrosion
Mechanical Properties

The work is accomplished in a variety of ways. Four ongoing data centers exist: Crystal Data, Alloy Phase Diagrams, Phase Diagrams for Ceramists, and Corrosion. Each of these has cooperative agreements linking its activities to major outside technical groups (Table 2). This ensures that the data center work addresses the needs of the U.S. research and technical communities. Projects are often jointly funded and, in some cases, substantial amounts of industrial support have been raised for these programs.

Table 2

Major NBS-Outside Data Agreements	
American Society for Metals	(Alloy Phase Diagrams)
American Ceramic Society	(Phase Diagrams for Ceramists)
International Centre for Diffraction Data-JCPDS	(Crystal Data)
Society of Plastics Engineers	(Polymeric Blend Phase Diagrams)
National Association of Corrosion Engineers	(Corrosion Data)

The Materials Properties Data program has a number of short-term evaluation projects that address specific data needs within the framework given in Table 3. These are done both inside and outside NBS. Often these represent pilot projects within new programs to demonstrate feasibility and types of output, to serve as models for larger efforts, and to get the programs going.

Table 3

OSRD Materials Properties Data Program

Structure and Characterization

- Crystallography
  - NBS Crystal Data Center
  - JCPDS - ICDD
  - Cambridge Crystallographic Data Centre
  - Cation-Nitrogen Distance (U. Ill. - Chicago)
- Surfaces
  - ESCA Data Project - Surfax (CA)
  - Ion Sputtering - NBS

Physical Properties

- Optical
  - Refractive Index - CINDAS (Purdue)
- Molecular Weight of Polymers - NBS

Phase Equilibria

- Alloys
  - NBS Alloy Phase Diagram Data Center
  - NBS/ASM Phase Diagram Program
    - Fe, Al, Ti - NBS
    - V, Nb - Ames
    - Cr - U. Alabama
    - Cu - Carnegie-Mellon
    - Rare Earths - Iowa State
    - Alkalis - Montreal
    - Actinides - LASL
- Ceramics
  - NBS Phase Diagrams for Ceramists Data Center
- Thermochemistry
  - Thermochemistry of Alloy and Elements - CINDAS (Purdue)

Corrosion

- NBS Corrosion Data Center
- NBS/NACE Corrosion Data Program
  - Stainless Steels in Aqueous Chlorides - Georgia Tech

Mechanical Properties

- Fracture Toughness - NBS
- Fatigue - John Deere and SAE
- Creep Rupture - Metal Properties Council
- Data Standardization - General Electric

Finally, a major part of the program is to help user groups define their evaluated data needs, set up programs to address them, and find necessary support. In the past year several such efforts have taken place, especially in the area of mechanical properties data.

Let us touch on the highlights within each component; new areas of activity will also be pointed out.

Structure and Characterization

The structure and characterization of solid materials are extremely important. The identification of unknown substances has always been a major use of evaluated data. The NBS Crystal Data Center has developed powerful techniques for rapidly identifying crystalline substances. Computer-readable databases supporting this work are being distributed, and it is hoped that they will be integrated into diffractometers soon. The NBS Data Center interaction with the International Centre for Diffraction Data-JCPDS (ICDD-JCPDS) continues. This past year the ICDD-JCPDS has had a research associate at the NBS center working on software to be used with the NBS Crystal Data Identification File. That software is now complete and ready to be distributed.

Surfaces as well as bulk materials have received a great deal of attention. Over the last 20 years, a number of techniques involving electron and photon spectroscopies have been developed to characterize surfaces, and the data generated are in need of evaluation. One project on ESCA data is underway, but many more are needed. During the last year, OSRD, working with the Surface Science Division in the Center for Chemical Physics, established a project on ion sputtering.

Physical Properties

A project evaluating optical data (refractive index) was completed this year by CINDAS. In addition, the first phase has been completed for a project on evaluating molecular weight data for polymers.

Phase Equilibria

NBS, through the Center for Materials Science (CMS) and OSRD, has three major programs for evaluating phase data for alloys, ceramics, and polymeric blends. These major programs are well integrated into the user communities, and significant progress was achieved in all three this year.

The Alloy Phase Diagram Center is the focal point of the NBS/American Society for Metals (ASM) joint program to evaluate all alloy phase diagrams. Over the last year, the Alloy Center has continued to exert vigorous technical leadership. The Bulletin of Alloy Phase Diagrams published over 50 new diagrams, and work on prototype databases continued. OSRD supports the program in two major ways: direct support of the data center and support of individual evaluation projects (see Table 3).

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The Phase Diagrams for Ceramists Data Center has been implementing their agreement with the American Ceramics Society (ACerS) for a joint program on evaluated data. ACerS has begun fund-raising efforts, and NBS data center has established vigorous programs in database graphics and thermodynamic modeling. In addition, new systems such as molten salts are receiving attention.

Phase data for polymeric blends are important in developing new and improved polymers. NBS and the Society of Plastics Engineers (SPE) are holding a workshop this fall on this subject which will help provide guidance for this work.

Performance Properties

Corrosion

The National Association of Corrosion Engineers (NACE) and NBS are now beginning projects under a cooperative agreement which will provide the technical community with evaluated corrosion data. The Metallurgy Division (CMS) and OSRD have established the NBS Corrosion Data Center to act as the technical focal point of this program. Several pilot projects have been started in both kinetic and thermodynamic areas. A major corrosion data workshop is planned for spring 1985.

Mechanical Properties

OSRD has been working closely with outside groups to address a variety of problems related to mechanical properties data. In particular, the Metal Properties Council (MPC) has developed a major effort to provide computerized access to materials property data. The Office has interacted strongly with this project and has developed a four-pronged effort involving data evaluation, data standardization, database creation, and user workshops.

The evaluation of mechanical properties data until now has been concentrated in areas of high technology such as nuclear power generation and aerospace. This past year, OSRD started several evaluation projects, working with groups such as SAE, MPC, and ASME.

Computer access to mechanical properties data will cause new problems with respect to standardization of data generation and reporting. Data on computers can quickly lose their pedigree, be combined incorrectly with inappropriate data, and misused in other ways. A recent OSRD study is being sent ASTM to spur rethinking present standards in this area.

The MPC materials property data network will involve linking together many databases on a variety of properties created by interested parties. For such a system to be useful, more databases must be created from the now existing published compilations. MPC and OSRD will work together to persuade publishers, societies, and other groups to begin building the needed databases more intensely.

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A key ingredient to success in this type of project is strong user input from the beginning. To this end, NBS and MPC have set up a series of user workshops addressing the needs in several application areas. The workshops outline detailed needs and will help pave the way for industrial acceptance and support of the system. In 1984, two workshops were held, the first for the ground vehicle industry and the second for the nuclear power industry.

Summary

Inherent in all the above activity is the need for increased resources. At present, OSRD has stretched its existing resources extremely thin. The industrial community has turned to OSRD for leadership, which OSRD is working to provide. A major effort thus will be mounted to attract from NBS and other government agencies the attention these activities deserve and to turn that attention into direct support.

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COMPUTERIZATION

B. B. Molino, Group Leader

The major commitment by the Office of Standard Reference Data to automate the internal operations of its data centers and to develop numerical databases for dissemination has continued throughout the past year. Progress has been made in many areas, as summarized below.

Computing Facilities

We are pleased to announce that after six years of effort, the Bureau has been successful in awarding a contract to upgrade its central computer facilities. Next March installation will begin on a Control Data Corporation Cyber 205 with a Cyber 855 front end and a high-speed network connecting the two. By this time next year, we anticipate this supercomputer being used by OSRD staff and by the data centers in all aspects of their automation efforts.

The OSRD Hewlett Packard 1000 computer facility has been enhanced with a printer capable of producing camera-ready copy and with a 404 megabyte disc drive. In addition, it is now connected to the NBS net. We are coordinating our efforts with the individuals using the HP 1000 in the Center for Chemical Physics and are increasing our library of available software, both purchased and developed in-house. OSRD as well as the CCP machines will be upgraded shortly to give three times the processing power and better turn-around to the users.

The office now has both an Apple and an IBM PC microcomputer. In addition to being used for administrative purposes, these machines will be available for experimentation concerning the distribution of Standard Reference Data for personal computers. Finally, we are now making use of our first word processor and expect to receive others shortly to automate our secretarial staff.

Publication Procedures

Conversion to the Bedford Composition System for computer typesetting of our publications is complete. We have already realized a reduction in the amount of processing required in this office as well as a reduced turnaround time and anticipate even greater efficiency when the specific manuals we are developing for use by the data centers are complete.

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Numerical Database Activity

The six NBS Standard Reference Databases presently available (listed in Table I) have generated considerable interest and a substantial number of leases. We have recently revised our pricing policy by reducing the annual lease fee for distributors, thus attracting on-line vendors to make the databases available at an acceptable price to traditional user groups in industry, universities, and Government.

Table I

NBS STANDARD REFERENCE DATABASE	On-line Availability
1. NBS/NIH/EPA/MSDC Mass Spectral Data Base	CIS, Questel
2. NBS Chemical Thermodynamics Data Base (NBS Tech Note 270)	CIS
3. NBS Crystal Data Identification File	CIS, CISTI
4. NBS Thermophysical Properties of Hydrocarbon Mixtures (TRAPP)	
5. Thermophysical Properties of Helium	
6. Interactive Fortran Program to Calculate Thermophysical Properties of Six Fluids	

One highlight was when we demonstrated these databases and their associated interactive software at the Ninth International CODATA Conference in June. From a terminal in Jerusalem, Israel, we communicated via ISRANET and TYMNET, through the Intelligent Gateway at Lawrence Livermore National Laboratory, to our own OSRD computer facility. Interest was high, and we have had requests to experimentally access our system, software, and databases.

We anticipate quite a few additions to this NBS Standard Reference Database Series in the near future. Among them will be the JANAF Tables and interactive programs to calculate the Steam Tables (as published in Haar, Gallagher, and Kell).

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Database Activities

Individual data centers continue to make great progress in their database efforts. Ongoing projects in this area are summarized in Table II.

Table II

OSRD Activities in Numerical Data Bases

Crystal Data

- NBS Crystal Data Identification File
- NBS Master Crystal Data File (with Cambridge, Bonn, Ottawa)

Chemical Thermodynamics
- Inorganic Compounds - NBS
- Organic Compounds - Texas A&M
- Temperature-dependent Inorganic (JANAF) - Dow Chemical

Phase Diagrams
- Alloy (with ASM)
- Ceramics (with ACerS)

Atomic Spectra
- Energy Levels
- Transition Probabilities

Kinetics of Chemical Reactions
- Combustion Reactions
- Atmospheric Reactions
- Photo-initiated (Fast)

Properties of Fluid Mixtures
- Hydrocarbons
- Polar Molecules
- Helium

Collision Cross-Sections
- Electrons
- Photons and Charged Particles

Several other major database activities deserve mention. The first is a cooperative bibliographic database project undertaken by OSRD and the data centers in the Center for Chemical Physics. Key individuals in both areas are coordinating efforts to design and standardize a minimum set of data elements. Programmers are cooperating in implementing the various aspects required to create the entire system, including screen routines for input and updating, and report generators. It is our goal to apply this system to other bibliographic files, and we have already helped other data centers link auxiliary files, when required.

Another major commitment now underway is the automation of the numeric files for the Atomic Energy Levels Data Center and the Atomic Transition Probabilities Data Center. The specification and design stage of a computerized database system of atomic spectroscopic data is now underway, including the description of data elements and their relationships, the formulation of user queries and output formats, the design of the file structure, and the development of mathematical algorithms for checking input data validity.

Reference Center Automation

All of our automated files of reference center holdings and JPCRD articles, including property and materials terms, have been transferred to the HP, and the file structure modified accordingly. This will greatly facilitate the preparation of indexes and publication lists and allow for greater ease in computer typesetting these products. In addition, there is now greater potential for on-line searching of these files. Future automation projects are being considered, such as more in-depth indexing.

Outside Interactions

OSRD continues to interact extensively with outside groups who wish to build numeric databases, and staff members take initiative in leading these efforts. Examples of cooperative efforts include working with The Metal Properties Council, with DOE in building a Materials Database System, with AIChE on the DIPPR project, and with such international groups as CODATA and IUPAC. These activities continue to be very fruitful.

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DATA CENTER AND PROJECT REPORTS

The following pages provide brief descriptions of the scope and activities of each of the continuing data centers and short-term projects within which the data evaluation and compilation work is carried out. The data centers are listed in alphabetical order by name. The short-term projects are categorized by the OSRD program area under which they are managed.

DATA CENTERS

ALLOY PHASE DIAGRAM DATA CENTER

Kirit Bhansali, Director
Center for Materials Science, NBS

The Alloy Phase Diagram Center collects, evaluates, and distributes phase stability data for metal alloy systems and is the technical coordinator for the NBS-ASM Alloy Phase Diagram Program.

The Center is responsible for the technical content and editing of the Bulletin of Alloy Phase Diagrams, a joint publication with the American Society for Metals. The Bulletin, now a bimonthly publication, has rapidly become the prime source of evaluated phase diagrams. Computer graphics software for phase diagrams has been developed and is used to help produce the Bulletin, as well as for input of data to the database.

A vigorous evaluation program for titanium systems, with support by ONR, is now well into its fourth year, and more than 44 titanium binary systems have been evaluated. Evaluation of aluminum systems has begun, supported in part by DARPA. In addition, work on iron systems supported in part by DOE is now in its second year, and five systems have been evaluated. During this evaluation effort, thermodynamic optimization programs have been enhanced and interfaced with the graphics software.

Work for designing and creating a database of phase information and ancillary data is underway. This is being done in close cooperation with the ASM. Two ASM Research Associates are working in the Center for development of a prototype database.

AQUEOUS ELECTROLYTE DATA CENTER

David Smith-Magowan, Manager
Center for Chemical Physics, NBS

The Center provides the chemical process and related industries with critically evaluated data on the thermodynamic properties of aqueous electrolyte solutions including activity and osmotic coefficients, excess and partial molar enthalpy, heat capacity and volume of solution, solubilities, EMF and equilibrium constants for reactions in solution. It also provides techniques for correlation and estimation of such properties and information services.

The Center is closely coordinated with the Chemical Thermodynamics Data Center, using its bibliographic resources and providing it with evaluated data on aqueous systems as needed. These centers share a computer facility.

A database of activity and osmotic coefficients and excess Gibbs energies has been compiled for approximately 400 aqueous binary

electrolyte solutions. The base contains coefficients for fitting equations for each electrolyte solution which can be used to calculate activity and osmotic coefficients at a selected molality. It is planned that thermal data will be added to this database, to permit calculation of activities at higher temperatures.

An extended Pitzer equation has been applied to the correlation of the data for 110 electrolyte solutions. All of these activities apply to 25°C.

Procedures have been developed to calculate the excess, apparent molar and partial molar properties of aqueous solutions which associate, hydrolyze or hydrate. Excess Gibbs energy, excess enthalpy and heat capacities can be calculated. These procedures are expected to provide a necessary base for extending the interpolative and predictive capabilities of the Center to higher temperatures, mixtures, and complexing ions.

A series of bibliographics on aqueous solutions of CO_2, H_2S, H_2SO_4, NH_3, $CuCl_2$, H_3PO_4, $ZnCl_2$, the "sour water" system and general sources of thermodynamic data have been prepared for DIPPR.

A study has been started analyzing the thermodynamics of the Krebs cycle, utilizing data on enzyme-catalyzed equilibria in solutions. Network analysis techniques developed by CTDC are being applied to calculate correlated values of Gibbs energies of formation for approximately 30 substrates that participate in the Krebs cycle.

A detailed analysis has been made of the thermodynamic data on vapor-liquid equilibria and ionization equilibria in the SO_2-water system. The result is improved thermodynamic parameters applicable over the temperature range 0 to 100 °C.

ATOMIC COLLISION CROSS SECTION DATA CENTER

Jean W. Gallagher, Director
Center for Basic Standards, NBS

The Center's aim is to compile, evaluate, and disseminate data concerning electron and photon collisions with atoms, simple molecules, ions, and low energy heavy particle collisions. Emphasis is given to electron-collisional excitation and ionization, heavy-particle energy transfer, photoionization, photodetachment, and photofragmentation.

In the past year the Center has collaborated with a number of visiting scientists and JILA staff members to produce evaluated data publications. Articles on (1) collisional energy transfer rates and lifetimes for diatomic halogens and (2) theoretical charge transfer cross sections for non-hydrogenic atoms and ions appeared in this year's issues of the Journal of Physical and Chemical Reference Data. An update to the Multiphoton Bibliography for 1981-82 was completed. Articles on proton impact ioniziation of gaseous targets and on charge transfer for hydrogen and deuterium atoms and ions with metal vapors are

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nearing completion. An article on partial-channel photoionization of molecules is in progress. Collision strengths for electron impact excitation of ions are being compiled for a report on that subject which will be particularly useful to the astrophysics community.

A database management system has been designed for the storage and retrieval of the bibliographic and numerical data of interest to this Center. The bibliographic data has been loaded, and loading of the numerical data has begun.

ATOMIC ENERGY LEVELS DATA CENTER

W. C. Martin, Director
Center for Radiation Research, NBS

The Center compiles, evaluates and disseminates data on energy levels and spectral lines of atoms and atomic ions. Reliable atomic spectroscopic data are essential in such areas as plasma diagnostics, laser physics and astronomy.

A major updating and extension of energy-levels compilations for the 235 spectra of the iron-group elements K through Ni (A=19-28) was completed and submitted for publication as a supplement to the Journal of Physical and Chemical Reference Data. An energy-levels compilation for the 15 phosphorus spectra is almost complete. A supplement to the Bibliography on Atomic Energy Levels and Spectra covering the period July 1979 through December 1983 is in press.

Work on compilations of energy levels of phosphorus and sulfur will continue as part of our project covering the Na-Ar row (Z=11-18). Such work will be extended to the elements copper through molybdenum (Z=29-42), beginning with molybdenum. Future efforts will also include a compilation of forbidden spectral lines of interest for plasma physics and astronomy; this work will be the first of a series of planned compilations of atomic spectral lines (wavelengths and energy-level identifications).

ATOMIC TRANSITION PROBABILITIES DATA CENTER

Wolfgang L. Wiese, Director
Center for Radiation Research, NBS

The Center's purpose is to compile, evaluate, and disseminate data on atomic transition probabilities and lifetimes of excited levels of atoms and atomic ions. Interpretation of fusion plasma diagnostic techniques is highly dependent on the availability of these data.

Revision and updating of atomic-transition-probability data for allowed lines in the elements scandium through nickel is nearly complete, and work on evaluating data on forbidden transitions in these elements is in progress. Critical reviews of Stark widths and shifts in neutral and ionized atomic species were processed for automatic

typesetting and are in press. A computerized database of bibliographic information on atomic energy levels, atomic transition probabilities, and atomic line shapes and shifts was designed; much of the implementation of input capability, as well as very limited retrieval and output capability, was completed in collaboration with the staff of OSRD.

Future plans call for completing the compilation of transition probabilities for scandium through nickel, at which point the major effort will be focused on the light elements hydrogen through neon, as well as selected heavy elements (such as Kr and Zr). It is also planned to complete work on both input and output capability for the bibliographic database system. Input of references on atomic transition probabilities will be initiated. Long-range plans include the design and development of a computerized database of critically evaluated data on atomic spectroscopic quantities.

CINDAS (Center for Information and Numerical Data Analysis and Synthesis)

C. Y. Ho, Director
Purdue Unviersity
West Lafayette, Indiana

This is a large data center which receives support from a number of sources. It compiles and evaluates data on transport properties, heat capacities, thermal expansion, and optical, electronic, and electrical properties for a wide range of substances. For OSRD, CINDAS has been involved in the compilation and evaluation of data on thermal conductivity and electrical resistivity of metals and alloys and the thermal conductivity, viscosity, and heat capacities of fluids.

The present OSRD project involves evaluated thermochemical data for alloys and elements.

CHEMICAL KINETICS DATA CENTER

J. T. Herron, Director
Center for Chemical Physics, NBS

The Data Center is concerned primarily with the evaluation of gas phase chemical kinetic data. A compilation of evaluated data on 250 reactions involved in the oxidation of methane has been completed. Work on the oxidation of methanol, which is an extension of the methane system, is complete and being prepared for publication (about 90 evaluated reactions). Evaluation of data on halogen containing species relevant to stratospheric chemistry was also completed.

Progress has been made on the development of a database management system. Schemes for handling inorganic and organic nomenclature are in place, the method for searching for chemical reactions complete, and test databases have been entered to the HP-1000 system.

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In the coming year, the combustion database will be expanded to include C_3 and some C_4 species, reaching a total of about 500 evaluated chemical reactions. Extension to larger organic (non-aromatic) systems will require the development of theoretical predictive models. Work on the stratospheric chemistry database will continue at a maintenance level. The inclusion of both evaluated databases into a searchable database system will be a major goal.

CHEMICAL THERMODYNAMICS DATA CENTER

David Garvin, Director
Center for Chemical Physics, NBS

The Center provides the chemical process and related industries with critically evaluated thermodynamically consistent data which can be used to establish the equilibrium constants and heats of reaction for important chemical reactions. These critically evaluated data also are used in the design and interpretation of research in physics, chemistry, biochemistry, geochemistry, environmental science, metallurgy and other fields where chemical interactions are important. The Center provides data describing the change in the chemical properties of substances as well as bibliographic reference services on thermochemistry. In particular, the Center provides enthalpies and Gibbs energies of formation, entropies, C_p in the standard state at 298.15 K and 1 bar, and enthalpies of formation at 0 K for inorganic substances and simple organic substances, and to a more limited extent transition properties, and thermal functions. The publication "The NBS Tables of Chemical Thermodynamic Properties" represents completion of a major activity of the Center. It lists 26,000 data values pertinent to 14,000 substances. The experience gained in this work is now being applied in an international cooperative program under the auspices of CODATA.

The Center is cooperating with four others to design an ongoing system for evaluating thermodynamic data. Together they have produced a set of prototype tables. These tables covering a number of compounds of calcium and some auxiliary substances serve three purposes. One, they demonstrate the feasibility of producing chemical thermodynamic tables through the cooperative activities of a number of data centers in accordance with the system outlined in CODATA Bulletin No. 47, "A Systematic Approach to the Preparation of Thermodynamic Tables." Two, they provide a model for a new generation of tables. Three, preparation of the tables has provided practical experience to those involved in the preparation of tables using a decentralized highly-automated system. Toward the end of 1984 these tables will be made available for review and comment by the thermochemical community.

Each year the Center surveys the thermodynamic literature and extracts pertinent data. These go into its master index of thermodynamic measurement. This information is published annually as the Inorganic Section of the Bulletin of Chemical Thermodynamics.

The Center is making a major effort in the further development of its techniques. A major purpose is full automation of the Center's activities. This will promote internal efficiency and flexibility and

pave the way for easier, more effective cooperation with other data projects. A standardized procedure has been established for entry of bibliographic data into the system and preliminary versions exist for reaction catalogs and for the extraction of data from experimental papers.

CORROSION DATA CENTER

G. M. Ugiansky, Director
Center for Materials Science, NBS

The Corrosion Data Center is the NBS component of a joint program between the National Association of Corrosion Engineers (NACE) and NBS; it is concerned with the collection, evaluation, and effective dissemination of corrosion data. The central focus of the program is the establishment of an evaluated corrosion database which can be easily computer-accessed to provide the user with the required data in any of a number of possible graphical or tabular formats.

Several pilot projects have been initiated in the areas of kinetic and thermodynamic corrosion data. In the kinetic area, the projects include atmospheric corrosion of structural alloys, localized corrosion of stainless steel and other alloys, and uniform corrosion of alloys in aqueous and non-aqueous media. In the thermodynamic area, efforts have been focused on the use of computers for the calculation and display of stability diagrams of the electrochemical potential-pH type known as Pourbaix diagrams.

These pilot projects will be expanded and others will be added as the program continues to expand. The projects are planned in close collaboration with the NACE Steering Committee on the NACE-NBS Corrosion Data Program. A NACE Research Associate at NBS is developing dissemination methods for each project, and the NACE Committee is developing funding from industry to support an enlarged corrosion data evaluation effort which will involve experts throughout the corrosion community.

CRYSTAL DATA CENTER

A. D. Mighell, Director
Center for Materials Science, NBS

The Crystal Data Center is concerned with the collection, evaluation, and dissemination of data on solid state materials. The Center maintains a databaase which includes crystallographic and chemical information on all types of substances with known unit cells. The materials fall into the following categories: organics, organometallics, metals, intermetallics, inorganics, and minerals. For each substance, the data include the cell parameters, the space group, compound name and formula, calculated density, critical comments, and literature reference.

Using the database building program developed by the Center, NBS*AIDS, the data for each compound are processed, evaluated, and put

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into standard form. Derivative parameters are calculated such as the reduced cell, empirical formula, and calculated density. All data are kept in a computerized master database around which all data center operations are based. For example, books and derivative computer files are derived directly from the master database. The data have many applications including identification and characterization of solid state materials.

It is projected that within two years the Center will have data on more than 100,000 compounds. To avoid duplication of effort in database building and dissemination, the Center collaborates with other data centers including the Cambridge Crystallographic Data Centre, the JCPDS-International Centre for Diffraction Data, the Metals Data Center, and the Inorganic Structural Data Center.

The combination of the Crystal Data File and its associated software, NBS*LATTICE, constitutes a major new analytical and research tool of use to every scientist who works with solid state materials. Every effort will be made to bring this invaluable resource to the scientific community including independent distribution, incorporation into on-line systems such as CISTI, and integration into diffractometer software.

DIFFUSION IN METALS DATA CENTER

John Manning, Director
Center for Materials Science, NBS

The Diffusion in Metals Data Center is concerned with data on diffusion rates and mass transport in metals and their alloys.

The Center has recently completed a second volume of critically evaluated data dealing with diffusion in copper alloy systems. This work was done under a cooperative agreement with the International Copper Research Association (INCRA) and is published as part of the INCRA series on the Metallurgy of Copper. It will be a companion to an earlier volume concerned with a different group of copper alloys.

The data center has a collection of more than 25,000 documents reporting data on diffusion. This large database is being entered onto an on-line system, which will allow maintenance, updating, and retrieval of the information as needed. Specialized bibliographies on selected diffusion will be prepared as the data are entered into the system.

FLUID MIXTURES DATA CENTER

Neil A. Olien, Director
Center for Chemical Engineering, NBS

The Center is organized to compile and evaluate data on the thermodynamic and transport properties of fluids and fluid mixtures. These properties include formulations for the density and other thermodynamic properties of pure fluids, the viscosity and thermal conductivity of pure fluids, and the same properties for fluid mixtures.

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The Center is also involved with the development of techniques to predict transport properties of pure fluids from thermodynamic and molecular data, to predict properties of mixtures from the properties of pure fluids, and to interpolate and extrapolate data for properties over a range of temperature, pressure, and -- in the case of the mixtures -- mole fractions.

A second volume to "Thermophysical Properties of Fluids" has been prepared. "Thermophysical Properties of Fluids II" covers the C_1-C_4 aliphatic hydrocarbons. The two volumes cover eleven fluids.

A paper on the mixture methane/ethane which discusses both the state-of-the-art of the data for mixtures and the correlation of their properties in detail is in press. The discussions have impact on all mixture data fitting problems.

Experimental PVT results on CO_2/N_2 and methanol have been reported. The latter will form a basis for a correlation.

Work is ongoing to document the equation of state and the transport properties of the lower hydrocarbons C_1-C_5. A paper on propane is in review.

We have initiated an inhouse data center to note and document papers on the properties of hydrocarbons and their mixtures.

FUNDAMENTAL CONSTANTS DATA CENTER

Barry N. Taylor, Director
Center for Basic Standards, NBS

The Center provides a centralized source of information on the fundamental physical constants and on closely related precision measurements. It participates in the periodic development under the auspices of CODATA of sets of "best" or recommended values of the fundamental physical constants by means of least-squares adjustments. The self-consistent best values of the constants resulting from an adjustment are required for computational purposes and often are the basis for other data compilations. The Center also publishes a quarterly preprint and reprint newsletter entitled "Preprints on Precision Measurement and Fundamental Constants" or PMFC; participates in the organization of conferences relating to the precision measurement-fundamental constants (PMFC) field; administers the NBS Precision Measurement Grant program; and participates in the work of various committees in the PMFC field.

The major activity of the Center during FY 84 involved working towards the completion of the 1983 least-squares adjustment of the constants. The set of best values resulting from this adjustment will replace the now nearly obsolete set resulting from the 1973 adjustment. The 1983 effort, like its 1973 predecessor, is being carried out by B. N. Taylor in collaboration with E. R. Cohen and under the sponsorship and guidance of the CODATA Task Group on Fundamental Constants. The Task Group met in August 1984 to review the progress made to date by

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Cohen and Taylor and to offer its suggestions regarding the new adjustment.

The principal focus of the Center during FY 85 will be the completion and publication of the 1983 least-squares adjustment. It is expected that a CODATA Bulletin giving the new set of recommended values will be published in early 1985 and that the lengthy paper giving the details of the adjustment will be submitted for publication before the end of the year.

ION KINETICS AND ENERGETICS DATA CENTER

Sharon G. Lias, Director
Center for Chemical Physics, NBS

Since the publication in 1969 of NSRDS-NBS 26, "Ionization Potentials, Appearance Potentials, and Heats of Formation of Gaseous Positive Ions," the Ion Kinetics and Energetics Data Center has been considered by the scientific public as the preeminent source of authoritative evaluated data on the thermochemistry of ions in the gas phase. The primary long range goals of the Data Center are to maintain up-to-date archives of data on ionization potentials, appearance potentials, heats of formation of positive ions, ion-molecule reaction-rate constants and equilibrium constants, and to publish authoritative evaluations of those data.

Recent publications and publications in process include (1) "Evaluated Gas Phase Basicities and Proton Affinities of Molecules; Heats of Formation of Protonated Molecules" by Sharon G. Lias, Joel F. Liebman, and Rhoda D. Levin, Journal of Physical and Chemical Reference Data, in presss, and (2) "Ion Thermochemistry" by S. G. Lias, J. E. Bartmess, J. F. Liebman, J. L. Holmes, F. P. Lossing, and R. D. Levin (a comprehensive and complete compilation of evaluated heats of formation of more than 3000 positive and negative ions, now being prepared to be published in the Journal of Physical and Chemical Reference Data).

Dr. J. E. Bartmess of the University of Tennessee has evaluated the data on thermochemistry of negative ions for the forthcoming publication on heats of formation of ions. He will permanently maintain computer-searchable up-to-date archives of anion thermochemistry as an activity of our data center.

An evaluated compilation of thermochemical data on ion clusters (R. G. Keesee and A. W. Castleman, Jr., "Thermochemical Data on Gas-Phase Ion-Molecule Association and Clustering Reactions," Journal of Physical and Chemical Reference Data, in press) is being incorporated into our data archives at the request of the authors; the maintenance and updating of this database will become a permanent activity of the Data Center, in collaboration with Dr. Michael Mautner of the Chemical Kinetics Division, CCP.

In addition to maintaining up-to-date archives on ion energetics and issuing periodic updating supplements to these publications, future plans include the initiation of work on an evaluated compilation of data on ion-molecule rate constants and reaction cross sections.

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JANAF THERMOCHEMICAL TABLES

Malcolm W. Chase, Jr., Director
Dow Chemical Company
Midland, Michigan

The JANAF Thermochemical Tables Center covers the thermodynamic properties for the crystal, liquid, and ideal gas state over a wide temperature range. Properties covered are heat capacity, entropy, Gibbs energy function, enthalpy, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant for formation of each compound from the elements in their standard reference states.

Published tabulations involve 35 elements and their compounds. The 35 elements are H, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, V, Cr, Fe, Co, Cu, Br, Sr, Zr, Nb, Mo, I, Cs, Ba, Ta, W, Hg, and Pb.

A revised and updated comprehensive edition of the JANAF Tables is being prepared for publication as a Supplement to the Journal of Physical and Chemical Reference Data.

The JANAF Center is one of the five centers involved in the preparation of the prototype CODATA Thermochemical Tables which are discussed in more detail under the Chemical Thermodynamic Data Center.

MOLECULAR SPECTRA DATA CENTER

Frank J. Lovas, Director
Center for Chemical Physics, NBS

The Center provides for the collection, evaluation, and dissemination of molecular spectral frequencies and other molecular constants. These are designed to aid in the analysis and identification of compounds and to permit assignment of a wide range of molecular properties. One phase of the Center's work emphasizes microwave spectra of interstellar molecules.

A manuscript on "Recommended Rest Frequencies for Observed Interstellar Molecular Transitions in the Microwave Region" is nearing completion. The evaluation of microwave data for the "Microwave Spectral Tables of Hydrocarbon Species" is nearly complete. Finally, an infrared spectral calibration atlas for the frequency range 500 to 720 cm^{-1} is in progress and employs high resolution spectra of OCS, N_2O and CO_2.

Next year the "Recommended Rest Frequency" paper will be published. A manuscript on the spectra of hydrocarbons and on the infrared spectral atlas will be prepared.

MOLTEN SALTS DATA CENTER

George J. Janz, Director
Rensselaer Polytechnic Institute
Troy, New York

The Center compiles, evaluates and disseminates data on thermophysical properties of molten salt systems. Properties covered include density, electrical conductivity, viscosity, surface tension and selected thermodynamic properties including the eutectic points of mixtures.

Recommended values for properties of an extensive list of single and binary molten salt systems have been published in the Journal of Physical and Chemical Reference Data. At the present time, a concise updated summary publication in equation form is being prepared. At the same time, the data files of the Center are being automated. This automation will assist with the preparation and publication of the summary publication and simplify future updating.

Efforts are also underway to produce interactive automated products. A searchable comprehensive file of eutectic points is nearing completion. Other automated files to give numerical data for density, conductivity, viscosity and surface tension are being prepared.

NATIONAL CENTER FOR THE THERMODYNAMIC DATA OF MINERALS

John L. Haas, Jr., Director
U. S. Geological Survey
Reston, Virginia

The Center compiles, indexes, and evaluates data on the thermodynamic and thermophysical properties of minerals, their synthetic analogs, and geologic materials. These data are important for geochemical purposes and useful industrially in the fields of metallurgy and the synthesis and production of inorganic chemicals.

In particular, the Center develops critically evaluated thermodynamic data for naturally occurring solid phases or their chemical end members. Properties considered are heat capacity, entropy, enthalpy, Gibbs energy, enthalpy and Gibbs energy of formation, molar volume, molar compressibility, and molar expansivity, all as functions of temperature, and phase diagrams of systems containing mineral phases. The Center cooperates closely with the Chemical Thermodynamics Data Center and the JANAF Thermochemical Tables Project.

Some recent activities have centered about properties of geologic structures suggested as burial sites for high-level nuclear wastes.

PHASE DIAGRAMS FOR CERAMISTS DATA CENTER

L. Cook, Director
Center for Materials Science, NBS

The Phase Diagrams for Ceramists Data Center is responsible for collecting and evaluating phase diagrams for inorganic, nonmetallic systems. More specifically, systems covered are: metal-oxygen systems, metal oxides, oxygen-containing radicals, halides, sulfides, and high-temperature ceramic systems containing gaseous components. Also covered are various combinations of these types of systems. The goals of the Data Center are twofold: (1) maintenance of an up-to-date computerized database containing both bibliographic and graphic data and (2) provision of this information to the user community in readily accessible form, including timely publication of hardbound volumes. The Phase Diagrams for Ceramists Data Center works closely with the American Ceramic Society, which is reponsible for the publication of "Phase Diagrams for Ceramists," a Data Center product.

During the current year, significant progress has been made in the computerization of the database. More than 3000 bibliographic entries have been keyboarded. A software package for efficient digitization, editing, and plotting of binary ceramic phase diagrams using a micro-computer-based system has been developed. The first 50 binary phase diagrams were plotted in camera-ready form using this system. Work has begun on development of a similar package for ternary systems, specifically designed for the most efficient use in this data center. Additionally, the task of evaluating diagrams for inclusion in Volumes 6 and 7 of the PDFC Series has progressed steadily.

During the next year, the momentum of the database computerization effort will be increased. It is expected that during this year funds from the ACerS fundraising activity will become available so that ACerS research associates can be hired to work at NBS and assist with the task of database development. With this additional manpower, coverage will be extended to include carbides, nitrides and borides, semiconductors, and aqueous systems. The utilization of thermochemical optimization and computer modeling methods in evaluation will be increased.

PHOTON AND CHARGED PARTICLE DATA CENTER

M. J. Berger, Director
Center for Radiation Research, NBS

The Center compiles, evaluates, and disseminates data on the interaction of ionizing radiation with matter. The data on photons and charged particles include single-scattering cross sections as well as transport data pertaining to the penetration of radiation through bulk matter.

Activities during the past year include the following: (a) Tabulations have been published of relativistic Hartree-Fock-Slater modified atomic form factors in all elements from Z = 1 to 100. These results are applicable to the coherent scattering of photons and

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electrons; (b) Tabulations have been published of the density-effect correction for the stopping power of charged particles, as a function of particle velocity, for 278 materials; (c) A method has been developed for the synthesis of reliable bremsstrahlung cross sections, using various fragmented theoretical and experimental results. A systematic tabulation of the bremsstrahlung cross section is in progress for all elements, Z = 1 to 100, at energies from 1 keV to 100 GeV. (d) Using a previously developed database of photon cross sections for scattering, absorption and pair production in elemental substances, software has been developed for calculating these cross sections in compounds of any specified composition, duly taking into account the absorption edges for all the atomic constituents. This software will be used for a planned set of tables of cross sections for compounds of interest in radiation dosimetry and metrology; (e) A magnetic tape containing electron stopping powers, ranges and bremsstrahlung yields has been delivered to OSRD, to be used as an NBS Standard Reference Database.

RADIATION CHEMISTRY DATA CENTER

Alberta B. Ross, Director
Radiation Laboratory, University of Notre Dame
Notre Dame, Indiana

The Center's purpose is to compile, evaluate, and disseminate rate parameters and related data on chemical reactions initiated by the interaction of ionizing and photon radiation with matter. Emphasis is placed on those reactions occurring in aqueous and liquid media. Support of the Center is shared by OSRD and the DOE Office of Basic Energy Sciences.

A manuscript on superoxide rate constants is in press. Other data compilations in progress include:

Triplet-triplet absorption spectra - representing more than 800 individual chemical species.

Intersystem crossing quantum yields - representing more than 200 chemical species.

One-electron reduction potentials

Actinide reactions

Transients from water

Several programs for automation of the Center are underway. These include programs to produce and prepare for publication tables of data indexes and reference lists. Programs for on-line searching of numerical data files are also being developed. A searchable on-line bibliographic data base is available to users of the Radiation Laboratory and is being installed on DOE/RECON at Oak Ridge.

Publication of the biweekly and cumulative bibliographies is being continued.

THERMODYNAMIC RESEARCH CENTER

K. R. Hall, Director
Texas A&M University
College Station, Texas

The Center provides critically evaluated data on a wide variety of thermodynamic and thermophysical properties of organic compounds. These include thermodynamic properties of organic materials, condensed-phase properties, transition points and properties, density and vapor pressure of liquids, and ideal gas and real gas properties.

The Center has continued its work on the thermodynamic properties of organic substances containing the atoms C, H and O in the C_1 - C_4 range. A substantial number of major industrial products and intermediates is included in this group. Entropies and enthalpies for the condensed phases of all substances in the group for which low-temperature heat-capacity data are available have been gathered and evaluated. A paper is in the publication process. In another part of the same project, ideal-gas thermal functions have been prepared for those molecules in the group for which sufficient data are available. A paper has been submitted to the Journal of Physical and Chemical Reference Data. A third portion of the work involves the thermochemistry of these substances. Available enthalpies of reaction (primarily enthalpies of combustion) and equilibrium constants are used to obtain enthalpies, Gibbs energies and entropies for the substances concerned over a range of temperatures and states. Some consideration is also being given to the magnitude of real-gas effects.

The Center is involved in reevaluating the enthalpies of combustion of the lower aliphatic hydrocarbons, and prepares the section on organic compounds for the Bulletin of Chemical Thermodynamics which is published annually.

THERMODYNAMIC RESEARCH LABORATORY

Buford D. Smith, Director
Washington University
St. Louis, Missouri

This Laboratory compiles and evaluates data on the vapor-liquid equilibrium, excess enthalpy, and excess volume of binary subcritical fluid mixtures and data on the vapor pressures, enthalpies of vaporization, saturated-liquid densities, and virial coefficients of pure fluids which are components of the mixtures. The laboratory is funded jointly by industry and the Office of Standard Reference Data (OSRD). It covers a wide range of fluid mixtures, but its work for OSRD is focused on hydrocarbon-hydrocarbon systems with carbon numbers C_2 - C_8 and mixtures of hydrocarbons with aliphatic alcohols.

Papers on the benzene-hexane and benzene-cyclohexane systems have been published and comprehensive papers on all other C_6 - C_6 systems have been prepared. Currently, work is being carried out on hydrocarbon-aliphatic alcohol systems.

CRITICAL COMPILATION OF MASS SPECTRAL DATA

Martin G. Robiette
Mass Spectral Data Centre
Nottingham, England
Source of Support: NBS

This project compiles, evaluates, and enters mass spectra into the Mass Spectral Database. The data are collected from the open literature and other sources, both public and private. Their quality is assessed through application of a quality index algorithm. The high-quality spectra are added to the database.

This year over 1500 new spectra have been delivered. They are combined with spectra from other sources such as the U.S. Environmental Protection Agency, and disseminated on magnetic tape to individuals, laboratories, and on-line vendors. They are also periodically published through supplements to the NSRDS-NBS series of publications.

COMPILATION OF ATOMIC WAVELENGTHS BELOW 2000 ANGSTROMS

Raymond L. Kelly
Spectroscopic Data Center, Naval Postgraduate School
Monterey, California
Source of Support: NSF

This project has completed a compilation of atomic spectral lines with wavelengths below 2000 A. A manuscript is being prepared for publication as a major supplement to the Journal of Physical and Chemical Reference Data. The compilation will cover the elements hydrogen through krypton.

In the future, this type of work will be done within the NBS Atomic Energy Levels Data Center. Increased NBS and OA resources have been obtained to allow the expansion in the Data Center.

K SHELL IONIZATION BY HYDROGEN AND HELIUM IONS

Gregory Lapicki
East Carolina University
Greenville, North Carolina
Source of Support: DOE

This project has been recently completed, and a preliminary manuscript entitled "K Shell X-ray Production by Hydrogen and Helium Ions in The Elements (Z= 4 to 92)," has been delivered. The work presents x-ray production cross sections along with comparisons to theoretical results.

Present plans call for publication in the Journal, "Atomic Data and Nuclear Data Tables."

DIGITIZATION OF THE COBLENTZ SOCIETY INFRARED DATABASE

William Strauss
Johns Hopkins Applied Physics Laboratory
Columbia, Maryland
Source of Support: EPA, NIH

This project has been established to digitize a printed database of 5000 evaluated reference infrared spectra of substances in the condensed phase. The purpose is to provide the beginning of a major computer-readable database of IR reference spectra.

A minicomputer-based digitization system at the Applied Physics Laboratory is being utilized to generate the spectra. APL personnel are also compiling the associated information which will accompany each digitized spectrum.

A magnetic tape containing the first few hundred spectra will be delivered shortly. This will provide a check on numerous aspects of the digitization process and general structure and usefullness of the system. The remainder of the database will be completed when the final tape format is approved.

SOFT X-RAY INTERACTIONS WITH MATTER

Martin Berger
Center for Radiation Research, NBS
Source of Support: DOE, NBS

A pilot project has been established within the Photon and Charged Particle Data Center, to compile and evaluate soft x-ray cross sections (100 eV to 10 keV). Requirements for these photon cross sections exist, for example, in the following fields: Lithography in the manufacture of integrated circuits, EXAFS method for determination of atomic distributions in amorphous materials, trace element analysis by x-ray emission spectroscopy, design of x-ray lasers, and calculation of x-ray and particle beam radiation effects.

Plans are to analyze the available data for those elements where the data is most complete, compare with best available theory, and investigate the validity of additivity, that is of generating cross sections for compounds as linear combinations of cross sections for atomic constituents, and to estimate the corrections for departure from additivity.

MEDICAL PHYSICS DATA BOOK (2nd edition)

Medical Physics Data Group, AAPM
Source of Support: AAPM, NBS

The American Association of Physicists in Medicine (AAPM) has requested that a second edition of the highly successful Medical Physics Data Book be produced for use by hospital physicists. The handbook, which provides physical and chemical data related to radiologic and nuclear diagnostic and therapeutic techniques, will be expanded to include new information in all existing areas as well as subjects such as nuclear magnetic resonance (NMR) imaging.

Work is carried out by the Medical Physics Data Group of the AAPM. This group was constituted by the Association to monitor important data requirements and respond to them.

DATA ON AQUEOUS ELECTROLYTES

R. Wood
University of Delaware
Newark, Delaware
Source of Support: NSF

This project is closely coordinated with the work of the Aqueous Electrolyte Data Center. It is concerned with the evaluation, correlation and prediction of data on the thermodynamic properties of aqueous electrolyte solutions. Methods for computerized transfers of various data files between Delaware and NBS are also being investigated.

A primary objective is the development of methods for expressing the thermodynamic properties of aqueous electrolyte solutions over a wide range of temperatures. Fits have been obtained for solutions containing $MgCl_2$, HCl and NaCl up to 200 K. Since the electrolytes are weak at the higher temperatures, the method involves chemical equilibria as well as electrostatic effects.

Studies have been made of techniques for computer transfer of data files between Delaware and the Aqueous Electrolyte Data Center at NBS.

DIPPR DATA PROJECTS

AIChE
New York, New York
Source of Support: NBS, Industry

DIPPR supports a number of data compilation, evaluation, and prediction projects with cooperative funding from industry and Government. In accordance with an agreement between NBS and AIChE, the parent organization of DIPPR, DIPPR and NBS will cooperate in a variety of ways in the production of critically evaluated data for industry.

NBS is involved with 3 DIPPR activities: the preparation of a data prediction manual, preparation of a data book on phase equilibria in aqueous electrolyte systems and a data compilation for industrially important chemicals. NBS supports the preparation of the data prediction manual and also the preparation of an automated version of the manual. The data book on aqueous electrolytes is being readied for publication. It will contain data and bibliographies prepared by NBS. NBS also supported the preparation of an interactive automated version of the data compilation which will, when completed, contain in excess of 1000 compounds.

EQUILIBRIUM AND TRANSPORT PROPERTIES OF POLYATOMIC GASES AND THEIR MIXTURES AT LOW DENSITY

J. Kestin. E. A. Mason
Brown University
Providence, Rhode Island
Source of Support: NSF

The investigators have devised techniques to determine the intermolecular potentials for simple molecules from thermodynamic data. In a previous project, these techniques were used to derive definitive data for the thermodynamic and transport properties of the noble gases and their mixtures at low densities. The results of this work have recently been published.

These techniques are now being applied to a somewhat more complex set of fluids: H_2, N_2, O_2, CO, CO_2, N_2O and CH_4. The intent is to provide definitive data on the equilibrium and transport properties of these gases and their mixtures in the region of low density.

PREPARATION OF POURBAIX DIAGRAMS FOR SELECTED SYSTEMS

Marcel Pourbaix
Belgian Center for Corrosion Study
Brussels, Belgium
Source of Support: DOE

Reports have been prepared on the influence of temperature and pressure on the chemical and electrochemical equilbria of the systems O, H, Fe, O-H, O-Fe, H-Fe, O-H-Fe, C, O-C, C-Fe, O-C-Fe. This project is part of a larger program on chemical equilibria involved in corrosion processes.

PROPERTIES OF POLAR FLUIDS

L. Haar, J. M. H. Levelt-Sengers
Center for Chemical Engineering, NBS
Source of Support: NBS

During this period, a long-term effort on the thermodynamic properties of water and steam came to a conclusion. The NBS/NRC Steam Tables were published by Hemisphere Publishing Company and the International Association for the Properties of Steam approved of the IAPS Formulation 1984 for the Thermodynamic Properties of Ordinary Water Substance for Scientific and General Use. The latter replaces the Provisional IAPS Formulation 1982 for the Thermodynamic Properties of Ordinary Water Substance for Scientific and General Use. Each of these presents a variation on the same basic equation and will give the same numerical results. The equation permits the calculation of the thermodynamic properties of water for 0°C to more than 2500°C and to pressures as high as 20 kbar.

The program has now been turned toward the properties of mixtures and to the H_2O/CO_2 mixture in particular. It is hoped that the techniques developed for water can be expanded to cover binary systems.

THERMOPHYSICAL PROPERTIES DATA FOR FLUIDS

J. V. Sengers
University of Maryland
College Park, Maryland
Source of Support: NSF

This project is concerned with the development of comprehensive formulations for the thermodynamic and transport properties of fluids. This includes formulations providing an accurate description of the behavior in the critical regions.

A detailed evaluation was made of formulations proposed for the thermodynamic properties, viscosity and thermal conductivity of H_2O and D_2O on behalf of the International Association for the Properties of Steam (IAPS). As a result of this evaluation drafts were prepared which will serve as the basis for IAPS releases in these areas, and papers documenting this work were published in the Journal of Physical and Chemical Reference Data.

Further progress was made in using the modern theory of critical phenomena to provide correct representation of thermophysical properties in the critical region.

CRITICAL EVALUATION OF HIGH TEMPERATURE KINETIC DATA

N. Cohen
Aerospace Corporation
Los Angeles, California
Source of Support: DOD and NBS

This project compiles and disseminates evaluated data sheets describing the high-temperature kinetics of selected chemical reactions found to occur in rockets and jets.

The data sheet format is now firmly established. A total of 34 data sheets have been compiled to date. In addition, several manuscripts have been written. Some have been published as internal reports, and the rest have or will appear in outside journals. One paper was published in the Journal of Physical and Chemical Reference Data.

An additional 27 data sheets are being prepared. Systems covered are:

H_2-O_2, hydrocarbon-O_2, hydrogen-halogen, metal-O_2, O_2 energy transfer, haloalkane-O_2, NH_3-O_2.

SOLUBILITY OF THE SPARINGLY SOLUBLE SALTS OF ZINC, CADMIUM, AND MERCURY IN WATER AND AQUEOUS SALT SYSTEMS

R. Lawrence Clever
Emory University
Atlanta, Georgia
Source of Support: NSF

Compilations containing evaluated data on the solubility of zinc, cadmium, and mercury salts in water and aqueous electrolyte solutions are being prepared. The anions of interest include the halides, sulfides, sulfates, phosphates, and carbonates at all temperatures and pressures. In addition, an annotated bibliography on all the other anions for which data are available is being assembled.

A manuscript on mercury salts has been submitted to the Journal of Physical and Chemical Reference Data and a bibliography on the solubility of zinc and cadmium salts has been completed. The compilation and evaluation of the data on the solubility of zinc and cadmium is progressing.

CRITICAL EVALUATION OF CHEMICAL KINETIC DATA FOR METASTABLE ELECTRONICALLY EXCITED SPECIES

K. Schofield
ChemData Corporation
Santa Barbara, California
Source of Support: DOE

A critical evaluation is being performed on the available chemical kinetic rate data for the gas phase reactions of selected electronically excited species. In all, 19 species are being reviewed. They include excited states for NH, O_2, CN, C_2, CH NO, I, and N_2. The data are being prepared in a format similar to a previous publication on the subject and will also indicate where additional data are required.

A CRITICAL REVIEW OF POLYCHLORINATED BIPHENYL PHYSICAL - CHEMICAL DATA OF ENVIRONMENTAL RELEVANCE

D. Mackay
University of Toronto
Ontario, Canada
Source of Support: DOE

A critical review of the relevant thermodynamic and transport properties of polychlorinated biphenyls is being carried out. Nine properties are being assessed and an attempt to correlate these properties with "chlorine number" is being made. These relationships will be used to predict property values for those substances where no experimental values exist. Data for approximately 50 related compounds will be produced and procedures will be established for further applications.

CATION-NITROGEN DISTANCE IN NITRIDES OF CRYSTALLINE COMPOUNDS

W. H. Baur
University of Illinois - Chicago Circle
Chicago, Illinois
Source of Support: NSF

This project is reviewing and evaluating cation radii for crystalline nitride compounds. It has been found for many crystalline materials that, for a given anion, the cation radius remains the same despite differences in bond types and other structural changes. This has led to useful results, based on an assumption of the additive nature of these radii. However, the cation radii do change for different anions. The cation radii for nitride systems will be reviewed, and an evaluated set of radii will be generated. The nitride compounds have been chosen because of their significance in ceramic materials.

CRYSTALLOGRAPHIC DATA FOR ORGANIC MATERIALS

O. Kennard
Cambridge Crystallographic Data Centre
Cambridge, England
Source of Support: NBS

The Cambridge Crystallographic Data Centre has had a continuing collaboration with the NBS Crystal Data Center. The Cambridge Centre supplies two key sets of information: (1) numerical crystallographic data and references for organic and organometallic materials, and (2) actual copies of all published crystallographic research in organic materials. The Cambridge Centre has begun to supply the organic entries for the NBS Master Data File in the appropriate format, a major step forward in creating this important file. From these entries, selected information will be used to update the NBS Crystal Data ID File, which is available for on-line use.

OSRD BINARY PHASE DIAGRAM EVALUATION PROJECTS

Rare Earth Alloys

K. A. Gschneidner
Iowa State University
Ames, Iowa
Source of Support: DOE

Copper Alloys

D. E. Laughlin
Carnegie-Mellon University
Pittsburgh, Pennsylvania
Source of Support: DOE

Vanadium and Niobium Alloys

J. F. Smith
Ames Laboratory of DOE
Iowa State University
Ames, Iowa
Source of Support: DOE

Titanium Alloys

J. Murray
National Bureau of Standards
Gaithersburg, Maryland
Source of Support: ONR

Alkali Metals

A. Pelton
Thermfact
Montreal, Canada
Source of Support: DOE

Chromium Alloys

J. P. Neumann
University of Alabama
University, Alabama
Source of Support: DOE

Actinide Alloys

D. Peterson
Los Alamos National Laboratory
Los Alamos, New Mexico
Source of Support: DOE

These evaluation projects are a major part of the National Bureau of Standards-American Society for Metals (ASM) joint program to provide reliable phase stability information to the U.S. materials community. The format of all projects is the same. For each binary system, a recommended phase diagram will be produced with explanatory text including evaluation of available experimental, crystallographic, and thermodynamic data. The outputs will be published first in the Bulletin of Alloy Phase Diagrams and, as larger numbers of systems are completed, in a series of monographs published by ASM.

The titanium, vanadium, and niobium projects are now in their fifth year, and the rare earth alloys and copper projects are in their fourth year. The chromium and actinide projects have just started. A substantial number of binary systems evaluations have been completed.

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REFERENCE DATA ON THE REFRACTIVE INDEX OF SELECTED OPTICAL MATERIALS

H. H. Li
CINDAS
Purdue University
West Lafayette, Indiana
Source of Support: DOE

This project has produced recommended reference values for the refractive index of optically important materials, especially those which are serious candidates for use in high-power laser windows and for solar energy applications. The materials to be surveyed include cadmium and zinc sulfides, selenides and tellurides, and certain oxides and halides. All published work on this subject will be reviewed and the data evaluated. A manuscript on these compounds is being published in the Journal of Physical and Chemical Reference Data.

ESCA DATA BASE PROJECT

Charles Wagner
Surfax Company
Oakland, California
Source of Support: NSF

Electron Spectroscopy for Chemical Analysis (ESCA) is a technique that has proved of wide importance in characterizing the surface composition of materials. The present project is concerned with creating a database of critically evaluated line energy data for ESCA. One interesting aspect of this project is the use of a personal computer in building the database.

CORROSION RATE DATA FOR STAINLESS STEEL

M. Marek
Georgia Institute of Technology
Atlanta, Georgia
Source of Support: NBS

This is a pilot project in the NBS/NACE corrosion data program. The objective is to compile and evaluate corrosion rate data for austenitic stainless steels in aqueous chloride solution and to organize the data in suitable formats for presentation and retrieval. An important part of this effort is to identify the parameters which are important for the evaluation of corrosion susceptibility of these steels.

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THERMODYNAMIC REFERENCE DATA OF ELEMENTS AND BINARY ALLOYS

Pramod D. Desai
CINDAS
Purdue University
West Lafayette, Indiana
Source of Support: NSF

A key component of the NBS/ASM phase diagram evaluation program is the use of modeling software to ensure thermodynamic consistency. This project focuses on compiling and evaluating the thermodynamic data for a selected number of elements and alloys for use by evaluators in the NBS/ASM program. It will initially concentrate on Fe, Al, and Ti alloys.

STANDARDS FOR COMPUTERIZATION OF MECHANICAL PROPERTY DATA

Jack Westbrook
General Electric
Schenectady, New York
Source of Support: Army

The move towards providing computer access to materials data such as mechanical properties has led to some potential problems caused by the ease with which computers can combine data from different sources. This project is examining these problems for a few mechanical properties of a small number of materials. The result will be a set of recommendations for new procedures and standards which can be the basis of broader activities by U.S. engineering standards groups and NBS.

SURFACE SPUTTERING YIELD PROJECT

Cedric Powell
National Bureau of Standards
Gaithersburg, Maryland
Source of Support: DOE and NBS

Sputtering techniques for depth profile are used in a number of methods to analyze compositional changes of materials at surfaces and interfaces. Many of these techniques have matured to being able to provide quantitative sputter depth profile information, yet the necessary data are not readily available in easy-to-use, evaluated form. This project will prepare a compilation of evaluated sputtering yield data for several ion species and energies for targets of pure elements.

POLYMER SOLUTION MOLECULAR WEIGHT AND VISCOSITY PROJECT

H. Wagner
National Bureau of Standards
Gaithersburg, Maryland
Source of Support: NBS

Many properties of high polymers are dependent on their molecular weight, so its proper measurement is essential for control and specification. A variety of methods have been developed to measure the molecular weight. One of the most valuable is that based on viscosity—an empirical relationship known as the Marck-Houwink equation. This project evaluates the empirically-determined constants used for linear polyethylene in five commonly used solvents as well as a number of theta solvents.

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PUBLICATIONS IN 1984

Journal of Physical and Chemical Reference Data, Volume 13

No. 1

Thermodynamic Properties of Aqueous Sodium Chloride Solutions
Kenneth S. Pitzer and J. Christopher Peiper

Refractive Index of ZnS, ZnSe, and ZnTe and Its Wavelength and Temperature Derivatives
H. H. Li

High Temperature Vaporization Behavior of Oxides I. Alkali Metal Binary Oxides
R. H. Lamoreaux and D. L. Hildenbrand

Thermophysical Properties of Fluid H_2O
J. Kestin, J. V. Sengers, B. Kamgar-Parsi, and J. M. H. Levelt Sengers

Representative Equations for the Viscosity of Water Substance
J. V. Sengers and B. Kamgar-Parsi

Atlas of the Schumann-Runge Absorption Bands of O_2 in the Wavelength Region 175-205 nm
K. Yoshino, D. E. Freeman, and W. H. Parkinson

Equilibrium and Transport Properties of the Noble Gases and Their Mixtures at Low Density
J. Kestin, K. Knierim, E. A. Mason, B. Najafi, S. T. Ro, and M. Waldman

No. 2

Evaluation of Kinetic and Mechanistic Data for Modeling of Photochemical Smog
Roger Atkinson

Rate Data for Inelastic Collision Processes in the Diatomic Halogen Molecules
J. I. Steinfeld

Water Solubilities of Polynuclear Aromatic and Heteroaromatic Compounds
Robert S. Pearlman, Samuel H. Yalkowsky, and Sujit Banerjee

The Solubility of Nitrogen and Air in Liquids
Rubin Battino, Timothy R. Rettich, and Toshihiro Tominaga

Thermophysical Properties of Fluid D_2O
J. Kestin, J. V. Sengers, B. Kamgar-Parsi, and J. M. H. Levelt Sengers

No. 3

Experimental Stark Widths and Shifts for Spectral Lines of Neutral Atoms (A Critical Review of Selected Data for the Period 1976 to 1982)
N. Konjevic, M. S. Dimitrijevic, and W. L. Wiese

Experimental Stark Widths and Shifts for Spectral Lines of Positive Ions (A Critical Review and Tabulation of Selected Data for the Period 1976 to 1982)
N. Konjevic, M. S. Dimitrijevic, and W. L. Wiese

A Review of Deuterium Triple-Point Temperatures
L. A. Schwalbe and E. R. Grilly

Evaluated Gas Phase Basicities and Proton Affinities of Molecules; Heats of Formation of Protonated Molecules
Sharon G. Lias, Joel F. Liebman, and Rhoda D. Levin

Isotopic Abundances and Atomic Weights of the Elements
Paul De Bièvre, Marc Gallet, Norman E. Holden, and I. Lynus Barnes

Representative Equations for the Thermal Conductivity of Water Substance
J. V. Sengers, J. T. R. Watson, R. S. Basu, B. Kamgar-Parsi, and R. C. Hendricks

No. 4

Ground-State Vibrational Energy Levels of Polyatomic Transient Molecules
M. E. Jacox

Electrical Resistivity of Selected Elements
P. D. Desai, T. K. Chu, H. M. James, and C. Y. Ho

Electrical Resistivity of Vanadium and Zirconium
P. D. Desai, H. M. James, and C. Y. Ho

Electrical Resistivity of Aluminum and Manganese
P. D. Desai, H. M. James, and C. Y. Ho

Standard Chemical Thermodynamic Properties of Alkane Isomer Groups
R. A. Alberty and C. A. Gehrig

Evaluated Theoretical Cross Section Data for Charge Exchange of Multiply Charged Ions with Atoms, II. Non-Hydrogenic Target Atoms
R. K. Janev, and J. W. Gallagher

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Heat Capacity of Reference Materials: Cu and W
G. K. White and S. J. Collocott

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry: Supplement II
D. Baulch, R. Cox, R. Hampson, J. Kerr, J. Troe, and R. Watson

Supplement

Heat Capacities and Entropies of Organic Compounds in the Condensed Phase
E. S. Domalski, William H. Evans and Elizabeth D. Hearing

Other Publications in NBS Series

Technical Activities 1983, Office of Standard Reference Data
Sherman P. Fivozinsky
NBSIR 84-2864

Definition of Recommended Values of Certain Thermodynamic Properties for the Ketones
Buford D. Smith and Ol Muthu
NBSIR 84-2811

Data Publications from Other Publishers

NBS/NRC Steam Tables
Lester Haar, John S. Gallagher, and George S. Kell
Hemisphere Publishing Corp., 1984

Crystal Data Determinative Tables, 3rd Edition, Vols. 5 and 6
Alan D. Mighell, et al
JCPDS-International Centre for Diffraction Data, 1984

Bulletin of Alloy Phase Diagrams, Vols. 4 and 5, 1984
L. A. Bennett, Editor
American Society for Metals, 1984

(Evaluations done by NBS Alloy Phase Diagram Data Center and OSRD-funded projects)

Fe-Os	Cu-O	Cr-Cs
Fe-V	Cu-Bi	Cr-K
Fe-Fr	Cu-Tl	Cr-Li
	Cu-Cr	Cr-Na
Al-Na	Cu-Br	Cr-Rb
Al-Sn	Cu-Pb	
Al-Bi		Cs-K
Al-Si	Ti-Zn	Cs-Rb
Al-Pb		K-Rb
Al-Ge	Ag-Rare Earths	

Bibliographies and Indexes from Other Publishers

Biweekly List of Papers on Radiation Chemistry and Photochemistry
Vol. 17, 1984
Radiation Chemistry Data Center

Biweekly List of Papers on Radiation Chemistry and Photochemistry
Annual Cumulation with Keyword and Author Indexes, Vol. 16, 1983
Radiation Chemistry Data Center

Bulletin of Chemical Thermodynamics, Vol. 27, 1984
Robert D. Freeman, Editor
IUPAC Commission on Thermodynamics and Thermochemistry

PUBLICATIONS SCHEDULED FOR 1985

Journal of Physical and Chemical Reference Data, Volume 14

No. 1

Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C_1 to C_4, Part 1. Properties of Condensed Phases
Randolph C. Wilhoit; Jing Chao; Kenneth R. Hall

Standard Chemical Thermodynamic Properties of Alkylbenzene Isomer Groups
Robert A. Alberty

Assessment of Critical Parameter Values for H_2O and D_2O
J.M.H. Levelt Sengers, T. Straub, K. Watanabe, and P. G. Hill

The Viscosity of Nitrogen, Oxygen, and Their Binary Mixtures in the Limit of Zero-Density
Wendy A. Cole and William A. Wakeham

The Thermal Conductivity of Fluid Air
K. Stephan and A. Laesecke

The Electronic Spectrum and Energy Levels of the Deuterium Molecule
Robert S. Freund, James A. Schiavone, and H. M. Crosswhite

No. 2

Microwave Spectra of Molecules of Astrophysical Interest. XXII Sulfur Dioxide (SO_2)
Frank J. Lovas

Evaluation of the Thermodynamic Functions for Aqueous Sodium Chloride from Equilibrium and Calorimetric Measurements Below 154°C
E. Colin W. Clarke and David N. Glew

The Mark-Houwink-Sakurada Equation for Linear Polyethylene
Herman L. Wagner

Carbon Monoxide Thermophysical Properties from 68 to 1000 K at Pressure to 100 MPa
Robert D. Goodwin

No. 3 and 4 (Tentative)

Reactivity of HO_2/O_2 - Radicals in Aqueous Solution
Benon H. J. Bielski, Diane E. Cabelli, Ravindra L. Arndi, and Alberta B. Ross

A Review and Evaluation of the Phase Equilibria, Liquid Phase Heats of Mixing and Excess Volumes, and Gas Phase PVT Measurements for Nitrogen & Methane
A. J. Kidnay, R. C. Miller, E. D. Sloan, and M. J. Hiza

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Thermochemical Data on Gas-Phase Ion-Molecule Association and Clustering Reactions
R. G. Keesee and A. W. Castleman, Jr.

The Homogeneous Nucleation Limits of Liquids
C. T. Avedisian

Viscosity and Thermal Conductivity of Dry Air in the Gaseous Phase
K. Kadoya, N. Matsunaga, and A. Nagashima

The Solubility of Mercury and Some Sparingly Soluble Mercury Salts in Water and Aqueous Electrolyte Solutions
H. Lawrence Clever, Susan A. Johnson, and M. Elizabeth Derrick

Thermal Conductivity of Aluminum, Copper, Iron, and Tungsten at Temperatures from 1 K to the Melting Point
J. G. Hust and A. B. Lankford

Standard Chemical Thermodynamic Properties of Alkylnaphthalene Isomer Groups
Robert A. Alberty and Theodore M. Bloomstein

Standard Chemical Thermodynamic Properties of Alkene Isomer Groups
Robert A. Alberty and Catherine A. Gehrig

Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C_1 to C_4. Part 2. Ideal Gas Properties
Jing Chao, Kenneth R. Hall, Kenneth N. Marsh, and Randolph C. Wilhoit

Computer Methods Applied to the Assessment of Thermochemical Data. Part 1. The Establishment of a Computerized Thermochemical Data Base As Illustrated by Data for Titanium Chlorides
S. P. Kirby, E. M. Marshall, and J. B. Pedley

Benzene Thermophysical Properties from 279 to 900 K at Pressures to 100 MPa
Robert D. Goodwin

Supplements

JANAF Thermochemical Tables, Third Edition
M. W. Chase, Jr., Editor

Atomic and Ionic Spectrum Lines Below 2000 Angstroms
Raymond L. Kelly

Atomic Energy Levels of the Iron Period Elements: Potassium Through Nickel
J. Sugar and C. Corliss

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NSRDS-NBS Series Publications Scheduled for 1985

Selected Tables of Atomic Spectra: A. Atomic Energy Levels - Second Edition; B. Multiplet Tables; O III
Charlotte E. Moore
NSRDS-NBS 3(11)

Data Publications Scheduled from Other Publishers in 1985

Medical Linear Accelerator Central Axis Depth-Dose Data
James A. Purdy, William B. Harms, and Sherman P. Fivozinsky

Bibliographies and Indexes Scheduled from Other Publishers in 1985

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Vol. 18. 1985
Radiation Chemistry Data Center

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Vol. 17. 1984
Radiation Chemistry Data Center

Bulletin of Chemical Thermodynamics, Volume 28, 1985
Robert D. Freeman, Editor
IUPAC Commission on Thermodynamics and Thermochemistry

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LIST OF ACRONYMS AND ABBREVIATIONS

AAAS	American Association for the Advancement of Science
AAPM	American Association of Physicists in Medicine (AIP)
ACerS	American Ceramic Society
ACS	American Chemical Society
AIAA	American Institute of Aeronautics and Astronautics
AIChE	American Institute of Chemical Engineers
AIME	American Institute of Mining, Metallurgical, and Petroleum Engineers
AIP	American Institute of Physics
API	American Petroleum Institute
APL	Johns Hopkins Applied Physics Laboratory
APS	American Physical Society
ASM	American Society for Metals
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
BAPD	Bulletin of Alloy Phase Diagrams
CAC	Center for Analytical Chemistry, NML, NBS
CAD	Computer-Aided Design
CAM	Computer-Aided Manufacturing
CAS	Chemical Abstracts Service
CBS	Center for Basic Standards, NML, NBS
CCE	Center for Chemical Engineering, NEL, NBS
CCP	Center for Chemical Physics, NML, NBS
CINDAS	Center for Information and Numerical Data Analysis and Synthesis, Purdue University
CIS	Chemical Information System
CISTI	Canada Institute for Scientific and Technical Information
CMS	Center for Materials Science, NBS
CODATA	Committee on Data for Science and Technology (ICSU)
CRR	Center for Radiation Research, NML, NBS
CSIN	Chemical Substances Information Network
DARPA	Defense Advanced Research Projects Agency
DECHEMA	Deutsche Gesellschaft fur chemisches Apparatewesen
DIPPR	Design Institute for Physical Property Data (AIChE)
DOD	U. S. Department of Defense
DOE	U. S. Department of Energy
EPA	U. S. Environmental Protection Agency
ESCA	Electron Spectroscopy for Chemical Analysis
EXAFS	Extended X-ray Absorption Fine Structure
FDA	Food and Drug Administration
FIZ	Fachinformationszentrum
FY	Fiscal Year
GPE	General Purpose Equipment
GPSDC	General Purpose Scientific Document Code
GRI	Gas Research Institute
HP	Hewlett-Packard
IAPS	International Association for the Properties of Steam
ICDD	International Centre for Diffraction Data (JCPDS)
ICSU	International Council of Scientific Unions
INCRA	International Copper Research Association
IUPAC	International Union of Pure and Applied Chemistry (ICSU)
JANAF	Joint Army, Navy, Air Force (historical acronym)

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JCAMP	Joint Committee on Atomic and Molecular Physical Data
JCPDS	Joint Committee on Powder Diffraction Standards
JCPDS-ICDD	JCPDS-International Centre for Diffraction Data
JILA	Joint Institute for Laboratory Astrophysics, NML, NBS-University of Colorado
MPC	Metals Properties Council
MSDC	Mass Spectral Data Centre (UK)
NACE	National Association of Corrosion Engineers
NAS	National Academy of Sciences
NBS	National Bureau of Standards
NCI	National Cancer Institute
NEL	National Engineering Laboratory, NBS
NIH	National Institutes of Health
NLM	National Library of Medicine
NML	National Measurement Laboratory, NBS
NMR	Nuclear Magnetic Resonance
NRC	National Research Council
NSF	National Science Foundation
NSRDS	National Standard Reference Data System
OA	Other Agency (Funding)
OMS	Office of Measurement Services, NML, NBS
ONR	Office of Naval Research
OSRD	Office of Standard Reference Data, NML, NBS
OSTP	Office of Science and Technology Policy
PDFC	Phase Diagrams for Ceramists Data Center
PL	Public law
PMFC	Precision Measurements - Fundamental Constants
PMS	Physical Measurement Services
RCDC	Radiation Chemistry Data Center
SAE	Society of Automotive Engineers
SPE	Society of Plastics Engineers
SRD	Standard Reference Data
SRM	Standard Reference Material
STRS	Scientific and Technical Research and Services (appropriated NBS funds)
TRAPP	Thermophysical Properties of Hydrocarbon Mixtures Database
UNESCO	United Nations Educational, Scientific, and Cultural Organization
USGS	United States Geological Survey

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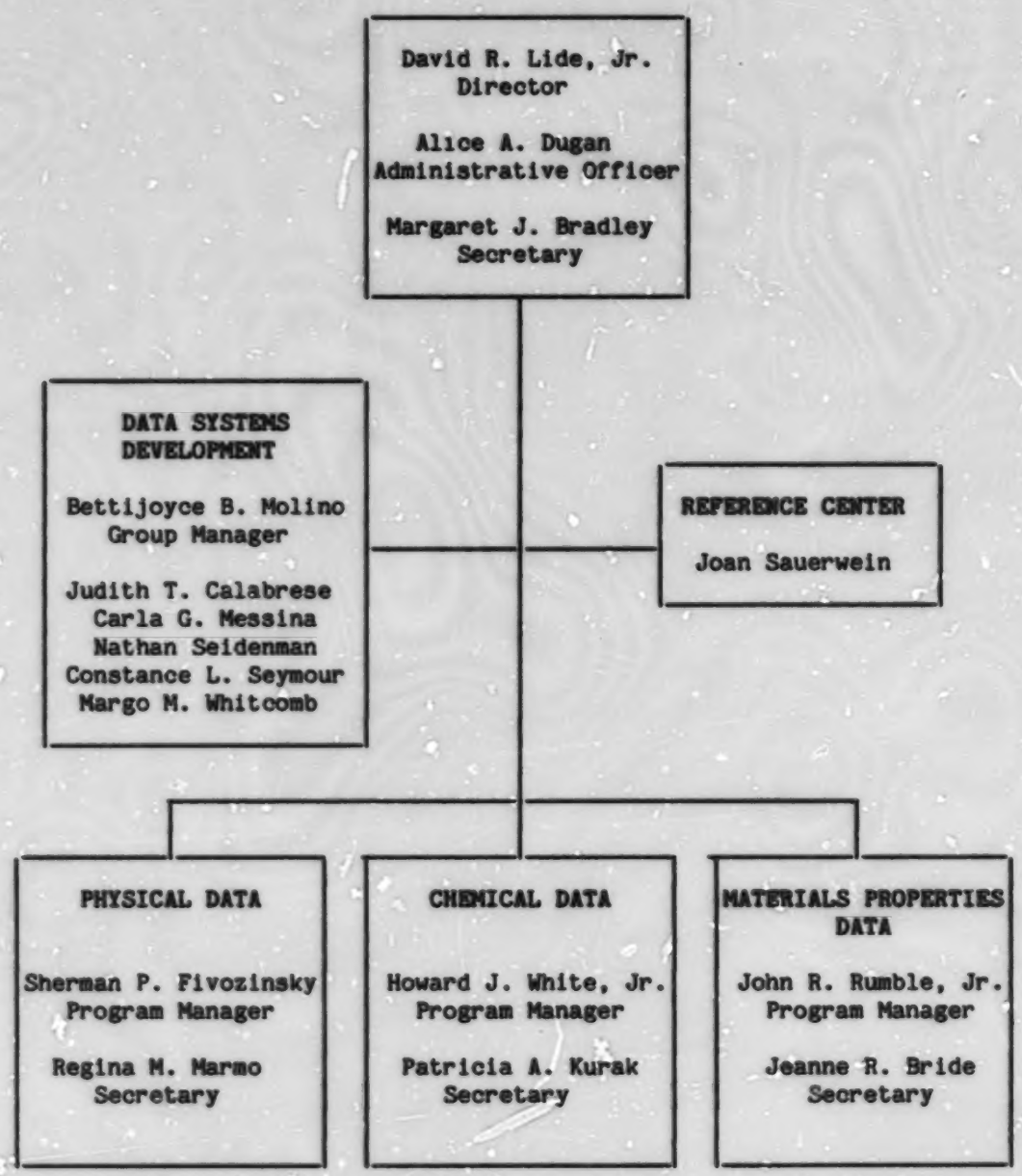
OFFICE OF STANDARD REFERENCE DATA



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Management of Chemical Data Program - kinetic, thermochemical, and thermophysical data

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Programming support for data center automation

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PUBLICATIONS BY OSRD STAFF

Report of a Workshop, The Effect of Computers on the Generation and Use of Technical Data, March 19-20, 1984, David R. Lide, Jr., Editor, NBSIR 84-2907

Tools for the Automated Handling of Evaluated Data, Bettijoyce B. Molino, Proceedings of the 9th International CODATA Conference (in press, North-Holland Publishing Company)

Effect of Electron Correlation in the Target Wavefunction on Electron-Molecular Scattering, J. R. Rumble, Jr., W. J. Stevens, and D. G. Truhlar, J. Phys. B. 17, 3151 (1984)

Why Can't We Access More Numeric Data via Computers, Proceedings of 5th National Online Meeting, New York, NY, April, 1984, J. R. Rumble, Jr.

Intelligent Gateways: Database Access - Challenges and Opportunities, Proceedings, 1st Pittsburgh Coal Technology Conference, Pittsburgh, PA, September, 1984, J. R. Rumble, Jr.

Database Management in Science and Technology, J. R. Rumble, Jr. and V. E. Hampel, Editors (North-Holland, Amsterdam, 1984)

Chapter 1. Data, Computers, and Database Management Systems
J. R. Rumble, Jr.

Chapter 4. Analysis and Display of Data in Science and Technology
J. R. Rumble, Jr. and N. L. Seidenman

INVITED TALKS AND PRESENTATIONS BY OSRD STAFF

Implications of Copyright on Accessibility and Dissemination of Numerical Data - An Update, Ninth International CODATA Conference, Jerusalem, Israel, June 1984
Sherman P. Fivozinsky

Attention to Data Needs in a Professional Society, Ninth International CODATA Conference, Jerusalem, Israel, June 1984
Sherman P. Fivozinsky

The Medical Radiation Depth - Dose Data Center in St. Louis, Missouri - A Status Report, Ninth International CODATA Conference, Jerusalem, Israel, June 1984
Sherman P. Fivozinsky

The Role of Computers in the Generation and Dissemination of Technical Data, 10th International Conference on the Properties of Steam, Moscow, USSR, September 1984
David R. Lide, Jr.

Introductory Remarks, Symposium on Standard Reference Data in Physical Chemistry, ACS Meeting - St. Louis, MO, April 1984
David R. Lide, Jr.

Automated NBS Standard Reference Databases, American Chemical Society National Meeting, St. Louis, MO, April 1984
Bettijoyce B. Molino

The Systems Approach: Standard Reference Databases, Northern Virginia Chapter of the Association for Systems Management, Arlington, VA, May 1984
Bettijoyce B. Molino

Tools for the Automated Handling of Evaluated Data, 9th International CODATA Conference, Jerusalem, Israel, June 1984
Bettijoyce B. Molino

Why Can't We Access More Numeric Data via Computers, National Online Meeting, New York, NY, April 1984
John R. Rumble, Jr.

Computerized Materials Data - A Progress Report, at Computerizing Materials Data - A Workshop for the Ground Vehicle Industry, Columbus, OH, April 1984
John R. Rumble, Jr.

Computerized Materials Data - A Progress Report, at Computerizing Materials Data - A Workshop for the Nuclear Power Industry, Knoxville, TN, May 1984
John R. Rumble, Jr.

Computerized Materials Data, Materials Committee, AIAA, Palm Springs, CA, May 1984
John R. Rumble, Jr.

Building Better Databases for Science and Technology, 9th International CODATA Conference, Jerusalem, Israel, June 1984
John R. Rumble, Jr.

Computerizing Materials Data - A Progress Report, 9th International CODATA Conference, Jerusalem, Israel, June 1984
John R. Rumble, Jr.

Numerical Data Bases for Materials Selection, Special Libraries Association, New York, NY, June 1984
John R. Rumble, Jr.

Online Databases for Materials Properties, Aluminum Association Standards Committee, Washington, DC, September 1984
John R. Rumble, Jr.

Computer Access to Materials Property Data, American Society for Metals, Technical Awareness Committee, Detroit, MI, September 1984
John R. Rumble, Jr.

Intelligent Gateways: Database Access - Challenges and Opportunities, 1st Pittsburgh Coal Technology Conference, Pittsburgh, PA, September 1984
John R. Rumble, Jr.

Online Access to Materials Property Data, Detroit Rubber Group, American Chemical Society, Detroit, MI, October 1984
John R. Rumble, Jr.

Comprehensive Consistent Thermodynamic Tables: A Report on Activities of CODATA, Calorimetry Conference McMaster University, Hamilton, Ontario, Canada, August 1984
Howard J. White, Jr.

Activities of the International Association for the Properties of Steam Between 1979 and 1984, 10th International Conference on the Properties of Steam, Moscow, USSR, September 1984
Howard J. White, Jr.

The Thermophysical Properties of Water and Steam, An Example of International Cooperation, International VDI-Seminar ORC/Heat Pumps - Technology at ETH Zurich, Switzerland, September 1984
Howard J. White, Jr.

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CIS Management Board

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American Institute of Physics (AIP) Publication Board

Committee on Nomenclature, ACS

Section Committee, Chemistry, AAAS

Petroleum Research Fund Advisory Board, ACS

Journal of Physical and Chemical Reference Data (Editor)

Committee on Data for Science and Technology of International Council of Scientific Unions (Secretary General)

Physical Chemistry Division, IUPAC (President)

Data Base Advisory Committee, IUPAC (Secretary)

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ASME Task Force on Materials Data for High Temperature Design and Analysis

Metal Properties Council Task Group of the National Materials Property Data Network
Chairman - User Needs Committee

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Task Group on Incentives for Evaluators, Numerical Data Advisory Board, NAS-NRC

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International Association for the Properties of Steam (Executive Secretary)

Task Group on Chemical Thermodynamic Tables (CODATA/ICSU) (Chairman)

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Engineering Sciences Data Unit Ltd. (Corresponding Member)

Research Committee on the Properties of Steam, American Society of Mechanical Engineers (Secretary)

Design Institute for Physical Properties Data (AIChE)
- Administrative Committee
- Technical Committee (non-voting)
- Liaison Committee
- Data Compilation Project Advisory Committee
- Electrolyte Data Project Advisory Committee

American Petroleum Institute Subcommittee on Technical Data (Advisor)

Public Law 90-396
90th Congress, H. R. 6279
July 11, 1968

An Act

To provide for the collection, compilation, critical evaluation, publication, and sale of standard reference data.

Be it enacted by the Senate and House of Representatives of the United States of America in Congress assembled,

Standard Reference Data Act.

DECLARATION OF POLICY

SECTION 1. The Congress hereby finds and declares that reliable standardized scientific and technical reference data are of vital importance to the progress of the Nation's science and technology. It is therefore the policy of the Congress to make critically evaluated reference data readily available to scientists, engineers, and the general public. It is the purpose of this Act to strengthen and enhance this policy.

82 STAT. 339

DEFINITIONS

82 STAT. 340

SEC. 2. For the purposes of this Act—

(a) The term "standard reference data" means quantitative information, related to a measurable physical or chemical property of a substance or system of substances of known composition and structure, which is critically evaluated as to its reliability under section 3 of this Act.

(b) The term "Secretary" means the Secretary of Commerce.

Collection and publication of standard reference data.

SEC. 3. The Secretary is authorized and directed to provide or arrange for the collection, compilation, critical evaluation, publication, and dissemination of standard reference data. In carrying out this program, the Secretary shall, to the maximum extent practicable, utilize the reference data services and facilities of other agencies and instrumentalities of the Federal Government and of State and local governments, persons, firms, institutions, and associations, with their consent and in such a manner as to avoid duplication of those services and facilities. All agencies and instrumentalities of the Federal Government are encouraged to exercise their duties and functions in such manner as will assist in carrying out the purpose of this Act. This section shall be deemed complementary to existing authority, and nothing herein is intended to repeal, supersede, or diminish existing authority or responsibility of any agency or instrumentality of the Federal Government.

Standards, etc. Publication in Federal Register.

SEC. 4. To provide for more effective integration and coordination of standard reference data activities, the Secretary, in consultation with other interested Federal agencies, shall prescribe and publish in the Federal Register such standards, criteria, and procedures for the preparation and publication of standard reference data as may be necessary to carry out the provisions of this Act.

Sale of reference data. Cost recovery.

SEC. 5. Standard reference data conforming to standards established by the Secretary may be made available and sold by the Secretary or by a person or agency designated by him. To the extent practicable and appropriate, the prices established for such data may reflect the cost of collection, compilation, evaluation, publication, and dissemination of the data, including administrative expenses; and the amounts received shall be subject to the Act of March 3, 1901, as amended (15 U.S.C. 271–278e).

31 Stat. 1449; Ante, p. 34.

U. S. copyright and renewal rights.

61 Stat. 655; 76 Stat. 446.

SEC. 6. (a) Notwithstanding the limitations contained in section 8 of title 17 of the United States Code, the Secretary may secure copyright and renewal thereof on behalf of the United States as author or proprietor in all or any part of any standard reference data which

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he prepares or makes available under this Act, and may authorize the reproduction and publication thereof by others.

(b) The publication or republication by the Government under this Act, either separately or in a public document, of any material in which copyright is subsisting shall not be taken to cause any abridgment or annulment of the copyright or to authorize any use or appropriation of such material without the consent of the copyright proprietor.

Appropriation.

SEC. 7. There are authorized to be appropriated to carry out this Act, $1.86 million for the fiscal year ending June 30, 1969. Notwithstanding the provisions of any other law, no appropriations for any fiscal year may be made for the purpose of this Act after fiscal year 1969 unless previously authorized by legislation hereafter enacted by the Congress.

Short title.

SEC. 8. This Act may be cited as the "Standard Reference Data Act."

Approved July 11, 1968.

LEGISLATIVE HISTORY:

HOUSE REPORT No. 260 (Comm. on Science and Astronautics).
SENATE REPORT No. 1230 (Comm. on Commerce).
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Vol. 114 (1968): June 13, considered and passed Senate, amended.
June 27, House concurred in Senate amendments.

GPO 88-139

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*The Office of Standard Reference Data is not involved at the present time in the administration or funding of these data centers but assists in making their outputs and services known to the scientific community.

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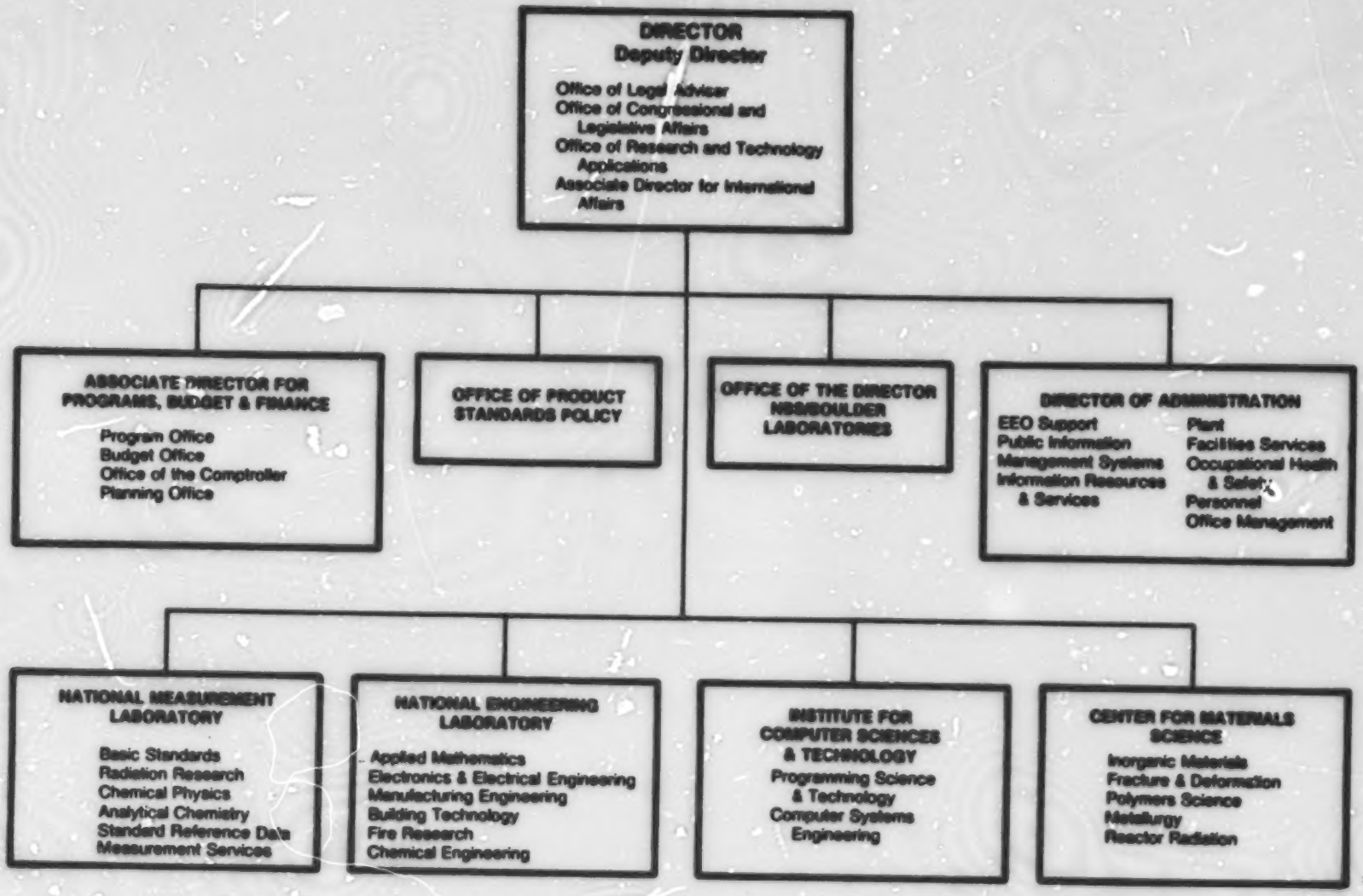

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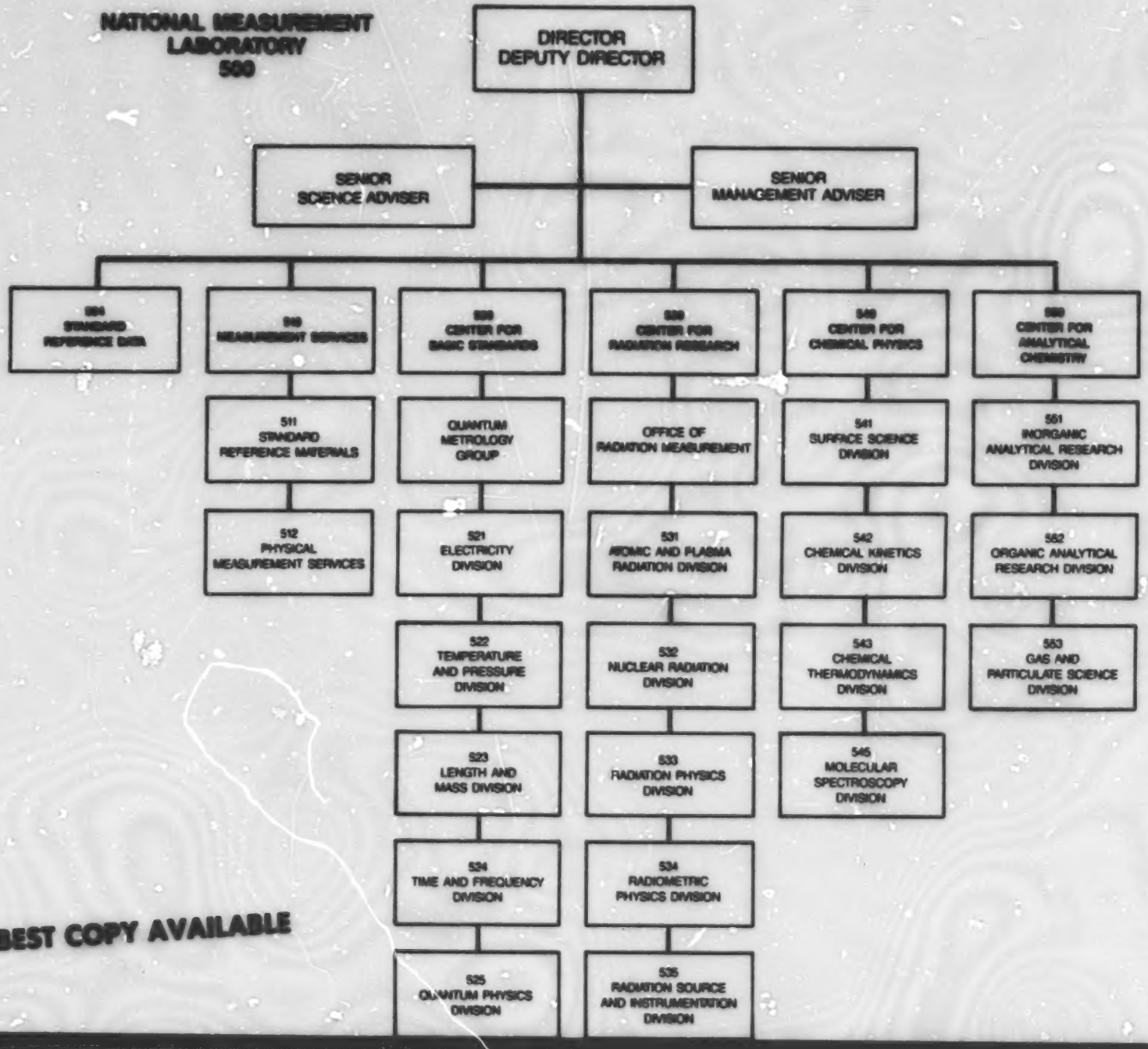
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10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

The Office of Standard Reference Data is one of two program offices in the National Measurement Laboratory, National Bureau of Standards. The Standard Reference Data Program develops and disseminates databases of critically evaluated physical, chemical, and materials properties of substances. These databases are available through NBS and private publications, on magnetic tape, and from online retrieval systems.

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the program for the year 1984.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

chemical data; data compilation; evaluated data; materials properties data; numerical database; physical data; standard reference data; technical activities 1984

13. AVAILABILITY

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